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U.S. DEPARTMENT OF COMMERCE / National Bureau of Standards

Standard X-ray Diffraction Powder Patterns

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No. 25-17
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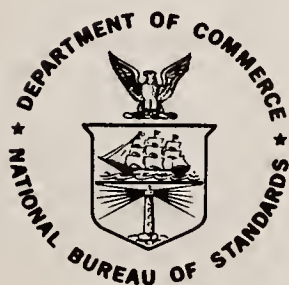
Standard X-ray Diffraction Powder Patterns Section 17—Data for 54 Substances

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Boris Paretzkin

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Diffraction Data

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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Previous work has been published as a book entitled Powder Diffraction Data from the Joint Committee on Powder Diffraction Standards Associateship at the National Bureau of Standards (1976) (JCPDS--International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081). The volume is sold with an accompanying search manual, and contains 949 card images of patterns of experimental data, published originally as Circular 539 (vols. 1-10) and Monograph 25, Sections 1-12, and most of Section 13.

Individual copies of the Circular and Monograph are still available and may be obtained from the National Technical Information Service, 5285 Port Royal Road, Springfield, VA 22161. If a publication listed below is identified with a number, it must be used in ordering. All are available in hardcopy or microfiche; the price is not fixed and will be furnished on request.

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ERRATA

Monograph 25

Section 16, pp. iii, 66, 176, 183: The corrected formula for sodium borate hydroxide hydrate (borax) is $\text{Na}_2\text{B}_4\text{O}_5(\text{OH})_4 \cdot 8\text{H}_2\text{O}$.

p. 1: In the 2nd column, last paragraph, line 5 from the bottom, the symbols should be $K\alpha_1$.

p. 129: In the paragraph "Structure", the space group should be $P2_1/c$.

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 17. --- Data for 54 Substances

by

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Eloise H. Evans and Boris Paretzkin
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and

Camden R. Hubbard and Simon J. Carmel
National Bureau of Standards

Standard x-ray diffraction patterns are presented for 54 substances. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings consistent with space group extinctions. The densities and lattice constants were calculated and the refractive indices were measured in some cases.

Key words: Crystal structure; lattice constants; powder patterns; reference intensities; standard; x-ray diffraction.

INTRODUCTION

The Powder Diffraction File is a continuing compilation of diffraction patterns gathered from many sources. Produced and published by the JCPDS--International Centre for Diffraction Data,¹ the File is used for identification of crystalline materials by matching d-spacings and diffraction intensity measurements. Under the partial sponsorship of the JCPDS, the program at the National Bureau of Standards contributes new data to this File. Our work also aids in the evaluation and revision of published x-ray data and in the development of diffraction techniques. This report presents information for 54 experimental patterns, and is the twenty-seventh of the series of ²Standard X-ray Diffraction Powder Patterns.

EXPERIMENTAL POWDER PATTERNS

CAS registry number. The Chemical Abstracts Service Registry Number is included, when available, to help identify the sample. This number forms the basis for computer aided searching of Chemical Abstracts.

Sample. The samples used to make NBS patterns were obtained from a variety of sources or were prepared in small quantities in our laboratory.

¹JCPDS--International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081. This Pennsylvania non-profit corporation functions in cooperation with the American Ceramic Society, the American Crystallographic Association, the American Society for Testing and Materials, The Clay Minerals Society, The Institute of Physics, the Mineralogical Association of Canada, the Mineralogical Society of America, The Mineralogical Society of Great Britain and Ireland, the National Association of Corrosion Engineers, and the Société Française de Minéralogie et de Cristallographie.

²See previous page for other published volumes.

Appropriate annealing or recrystallization of the samples improved the quality of most of the patterns. A check of phase purity was provided by indexing the x-ray pattern.

Optical data. When reported, optical measurements were made by grain immersion methods, in white light, using oils standardized in sodium light, in the refractive index range 1.49 to 2.1 [Hartshorne and Stuart, 1970].

The names of the sample colors were selected from the ISCC-NBS Centroid Color Charts [1965].

Interplanar spacings. For spacing determinations, a shallow holder was packed with a sample mixed with an internal standard. Choice of the standard was determined by the need for low angle and unobstructed reflections. The amount of standard was estimated so that the intensity of its strongest peak would be about equal to the intensity of the strongest peak of the sample.

To avoid errors associated with aberrations at the very top of the peaks, the readings of 2θ were taken at positions about 20% of the way down from the top, and in the center of the peak width. The $K\alpha_2$ peaks were occasionally read to assist in establishing a $K\alpha_1$ peak position, but $K\alpha_2$ peaks were not reported.

At low angles, $K\alpha_1$ and $K\alpha_2$ peaks were unresolved for both the sample and the internal standard. The internal standard corrections were established from the theoretical values for $K\alpha_1$ and were applied to the unresolved low angle peaks, as well as to the resolved $K\alpha_1$ peaks in the higher angle regions. If the internal standard correction varied along the length of the pattern, linear interpolations were used.

The internal standards used were of high purity (99.99%). The lattice constants used for them at 25 °C are given in Table 1; the 2 θ angles were computed using cell dimensions uncorrected for index of refraction.

Table 1

| Calculated 2 θ Angles, CuK α_1 λ = 1.540598Å | | | |
|--|----------------------------|-----------------------------|-----------------------------|
| hk ℓ | W a=3.16524Å ±.00004 | Ag a=4.08651Å ±.00002 | Si a=5.43088Å ±.00004 |
| 110 | 40.262 | | |
| 111 | | 38.112 | 28.443 |
| 200 | 58.251 | 44.295 | |
| 211 | 73.184 | | |
| 220 | 86.996 | 64.437 | 47.303 |
| 310 | 100.632 | | |
| 311 | | 77.390 | 56.123 |
| 222 | 114.923 | 81.533 | |
| 321 | 131.171 | | |
| 400 | 153.535 | 97.875 | 69.131 |
| 331 | | 110.499 | 76.377 |
| 420 | | 114.914 | |
| 422 | | 134.871 | 88.032 |
| 511/333 | | 156.737 | 94.954 |
| 440 | | | 106.710 |
| 531 | | | 114.094 |
| 620 | | | 127.547 |
| 533 | | | 136.897 |
| 444 | | | 158.638 |

The internal standard Si powder is available as Standard Reference Material 640 [1974]. The lattice constant for the Si was refined from multiple powder data measurements made with tungsten as an internal standard [Swanson et al., 1966]. Single crystal cell parameter data were also collected. The lattice parameters from the two methods agreed within three parts in 10⁵ [Hubbard et al., 1975]. D-spacing results using SRM 640 will be in agreement with patterns recorded in this series of monographs since 1966.

All of our spacing measurements were recorded at 25 ± 1 °C on a diffractometer equipped with a focusing graphite or lithium fluoride crystal monochromator located between the sample and the scintillation counter. Pulse height discrimination was used as well. All measurements were performed using copper radiation: $\lambda(\text{CuK}\alpha_1, \text{peak}) = 1.540598\text{\AA}$ [Deslattes and Henins, 1973].

Structure, lattice constants. The space groups were listed with short Hermann-Mauguin symbols as well as the space group numbers given in the International Tables for X-ray Crystallography, Vol. I [1952].

Orthorhombic cell dimensions were arranged according to the Dana convention $b > a > c$ [Palache et al., 1944]. Monoclinic and triclinic lattice constants were transformed if necessary in order to follow the convention of Crystal Data [1973].

A computer program [Evans et al., 1963] assigned hk ℓ s and refined the lattice constants.

Cell refinement was based only upon 2 θ_{obs} values which could be indexed without ambiguity. The program minimized the value $\sum(\theta_{\text{obs}} - \theta_{\text{calc}})^2$. The estimated standard deviations (e.s.d.'s) of the reciprocal cell parameters were determined from the inverse matrix of the normal equations. The program calculated the e.s.d.'s of the direct cell constants by the method of propagation of errors. Since 1973, the e.s.d.'s derived by the computer program have been increased by 50% in order to reflect more truly the uncertainty in the lattice constants. A similar increase should also be applied to all lattice constants in earlier publications of this series. The e.s.d.'s in the least significant figures are given in parentheses following the lattice constants.

In indexing cubic patterns, for a given reflection multiple hk ℓ 's were not utilized in the refinement or reported. Instead, the single appropriate index having the largest h was listed. The number of significant figures reported for d-values varied with the symmetry and crystallinity of each sample.

The number of significant figures at any reported d-value was derived from the average error in $|2\theta_{\text{obs}} - 2\theta_{\text{calc}}|$ and $\Delta d/d = -\cot\theta \Delta\theta$. With these conditions, the rounding of any specific d at the given number of significant digits yielded an error in its corresponding 2 θ which was less than the average error in 2 θ .

Densities. These were calculated from the specified lattice constants, the Avogadro number 6.0220943×10^{23} [Deslattes et al., 1974] and 1977 atomic weights published by the International Union of Pure and Applied Chemistry [1979].

Figure of merit. Several figures of merit ratings are available for assessing indexed powder data. M_{20} [de Wolff, 1968] is a criterion for the reliability of the unit cell and indexing. A value of $M_{20} > 10$ will guarantee the essential correctness of the indexing provided there are not more than 2 spurious lines ($X_{20} < 2$) [de Wolff, 1968]. In general, patterns reported in this publication had $M_{20} > 20$ and $X = 0$. M_{20} was specified for any pattern indexed with a cell derived only through computer indexing from powder data, without further confirmation.

The accuracy and completeness of measured interplanar spacings was conveniently reported as F_N [Smith and Snyder, 1979]. The format used in this publication was $F_N = \text{overall value} (|\Delta 2\theta|, N_{\text{poss}})$, where N , the number of observed reflections was chosen as 30, or the maximum number of lines of the pattern if the entire pattern had fewer than 30 lines. The "overall value" was the figure of merit, F_N , as defined by Smith and Snyder [1979], and $|\Delta 2\theta|$ was the average absolute magnitude of discrepancy between observed and calculated 2 θ values for each reported hk ℓ . N_{poss} was the number of diffraction lines allowed in the space group, up to the N^{th} observed and indexed line. Co-positional lines such as the cubic 221 and 300 are counted as one possible line.

Intensity measurements. It was found that samples which gave satisfactory intensity patterns

usually had an average particle size smaller than 10 μm , as recommended by Alexander et al. [1948]. In order to avoid the orientation effects which occur when powdered samples are packed or pressed, a sample holder was made that had in its top face a rectangular cavity which extended to one end of the holder. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall (see Figure 1), and the powdered sample was allowed to drift into the end opening while the holder was held in a vertical position. With the sample holder returned to a horizontal position, the glass slide was carefully removed so that the sample could be exposed to the x-ray beam (see Figure 2). If the sample powder did not flow readily, or was prone to orient excessively, approximately 50 volume percent of finely ground silica-gel was added as a diluent. Occasionally, a rotating sample holder was used instead. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentages of the strongest line.

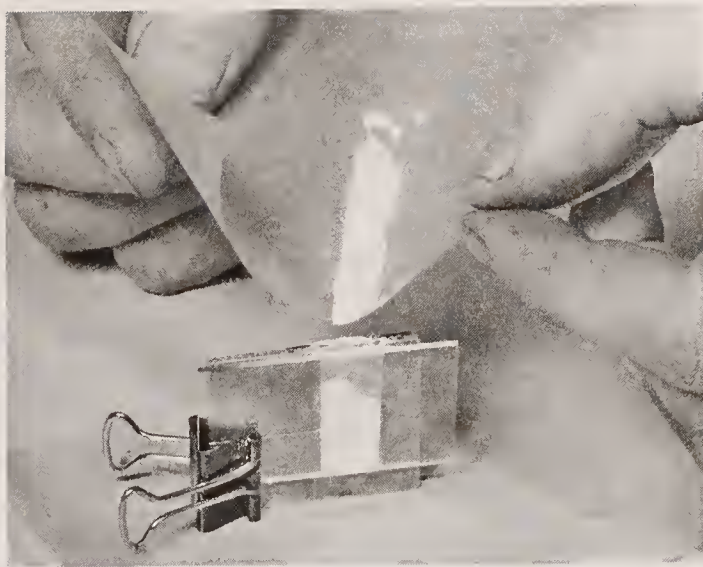


Figure 1.

As a check on reproducibility, each sample was mounted at least 3 times. The intensity values were determined for each of the mountings. Theta-compensating (variable divergence) slits were sometimes used to gather the intensity data. In that case, the average $I(\text{comp})$ for each spacing was converted to an equivalent fixed slit value, using the approximate equation:

$$I(\text{fixed}) = \frac{I(\text{comp})}{\sin \theta}$$

The reported I^{rel} value for each observed spacing was the scaled average of the separate measurements, rounded to the nearest integer. The estimated standard deviation, σ , in the relative intensity values was calculated from the values of the five strongest lines, excluding the line with $I = 100$.

$$\sigma_i^2 = \frac{1}{n-1} \sum_{j=1}^n (I_j^{\text{rel}}(k) - \langle I \rangle_j)^2$$

and

$$\sigma = \left\{ \frac{1}{m} \sum_{i=1}^m \sigma_i^2 \right\}^{\frac{1}{2}}$$

where .

m is the number of strong lines (usually 5), and

n is the number of independent observations i , per line.

Where conversion of intensities for effects of theta-compensating slits was required, each σ_i was multiplied by the conversion factor

$$f = \frac{I(\text{comp})}{I(\text{fixed})}$$

Reference Intensity Ratio, I/I_{corundum} .

The reference intensity ratio, I/I_c , has been defined as the direct ratio of the intensity of the strongest reflection of a sample, to the intensity of the reflection 113 (hexagonal) of corundum ($\alpha\text{-Al}_2\text{O}_3$) [Visser and de Wolff, 1964]. In this publication the ratios I/I_c were tabulated for copper $K\alpha$ radiation, for a 1:1 mixture



Figure 2.

by weight of the sample and corundum. Occasionally I/I_c was not determined because it was not feasible.

A procedure has been adopted, to achieve greater statistical accuracy [Hubbard and Smith, 1977]. For any weight fractions of sample and corundum, x_s and x_c ($x_s = 1 - x_c$), the intensities for reflection \underline{h} of the sample and \underline{k} of corundum were measured for several combinations of \underline{h} and \underline{k} usually within the same region of 2θ , to provide indications of possible preferred orientation, extinction, or other systematic errors. The reference intensity ratio is then given by

$$\frac{I(h_o)}{I_c(113)} = \frac{x_c}{x_s} \cdot \frac{I_c^{\text{rel}}(\underline{k})}{I^{\text{rel}}(\underline{h})} \cdot \frac{I(\underline{h})}{I(\underline{k})}$$

and (h_0) indicates specifically which reflection was chosen for tabulation purposes. For each of our patterns, the reflection (h_0) will be the one with $I = 100$ since only copper radiation was used. Typically, at least 3 sets of reflections and 2 mountings of the mixture were used to obtain 6 or more values for the reference intensity ratio, I/I_c . These values yield the tabulated average $\langle I/I_c \rangle$. From these data, the estimated deviation, Δ , was obtained from

$$\Delta = \frac{\sum_{i=1}^n \left| (I/I_c)_i - \langle I/I_c \rangle \right|}{n}$$

where n is the number of measurements of the reference intensity ratio. The estimated deviation in the least significant figures is given in parentheses.

Format of tables. The printing of the data has been computerized. Superimposed reflections were treated in one of two ways. If a d-spacing had only two possible indices, an \underline{M} was added to the d-spacing which was repeated on the next line, but with the second index. However, if there were more than two possible indices, a plus sign was used in like manner. In both cases, the composite intensity was printed only once and aligned with the first reflection. The symbol "1L" in the intensity column was used to indicate "less than 1".

UNITS

In this publication the Ångström unit ($1\text{Å} = 100\text{ pm}$) was selected for presentation of the d-spacings and lattice parameters to maintain consistency with (a) the earlier publications of Standard X-ray Diffraction Powder Patterns (Circular 539 volumes 1-10 and Monograph 25 sections 1-16), (b) the publications of the International Union of Crystallography: *Acta Crystallographica* and the *Journal of Applied Crystallography*, and (c) the continuing publication of cards and search manuals of the Powder Diffraction File (now consisting of over 33,000 entries). The PDF search manuals are based on the d-spacings in Å of the three strongest lines. Consistent with the choice of the Å unit for length, the volume of the unit cell is expressed in Å³ ($1\text{Å}^3 = 1 \times 10^{-30}\text{ m}^3$). Densities are reported in g/cm³ ($1\text{ gm/cm}^3 = 10^3\text{ kg/m}^3$).

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We would like to thank Carolyn Wingo of the JCPDS Associateship for her assistance, particularly for keyboarding the data and helping with the proofreading of this manuscript. Appreciation is also expressed to the Text Editing Facility of the National Measurement Laboratory of NBS for typing the manuscript.

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Aluminum Borate, $\text{Al}_{18}\text{B}_4\text{O}_{33}$

CAS registry no.
12005-61-7

Sample

The sample was prepared by heating a 1:1 mixture of Al_2O_3 and H_3BO_3 together at 1250 °C. The compound was later annealed at 1500 °C.

Color

Colorless

Structure

Orthorhombic, Amam (63), $A2_1am$ (36), or Ama2 (40), $Z = 1$ [Scholze, 1956]. Baumann and Moore [1942] reported data for this phase. Although the lattice constants were in good agreement with NBS constants, their pattern does not index on the given cell.

Lattice constants of this sample

$a = 7.6874(8) \text{ \AA}$
 $b = 15.0127(15)$
 $c = 5.6643(6)$

$a/b = 0.5121$

$c/b = 0.3773$

Volume

653.70 \AA^3

Density

(calculated) 2.685 g/cm^3

Figure of merit

$F_{30} = 65.2(0.010, 45)$

Reference intensity

$I/I_{\text{corundum}} = 1.27(5)$

Additional pattern

1. PDF card 9-248 [Scholze, 1956]

References

Baumann, H. N., Jr. and Moore, C. H., Jr. (1942). J. Amer. Chem. Soc. 25, No. 14, 391.
Scholze, H. (1956). Z. Anorg. Allg. Chem. 284, 272.

| CuK α_1 γ = 1.540598 Å; temp. 25±1 °C | | | | | |
|---|------------------|-----|---|---|----------------|
| Internal standard Ag, a = 4.08651 Å | | | | | |
| d(Å) | I ^{rel} | hkl | | | 2 θ (°) |
| $\sigma = \pm 3$ | | | | | |
| 7.52 | 1 | 0 | 2 | 0 | 11.76 |
| 5.375 | 100 | 1 | 2 | 0 | 16.48 |
| 5.301 | 18 | 0 | 1 | 1 | 16.71 |
| 4.365 | 52 | 1 | 1 | 1 | 20.33 |
| 3.846 | 8 | 2 | 0 | 0 | 23.11 |
| 3.750M | 16 | 0 | 4 | 0 | 23.71 |
| 3.750M | | 0 | 3 | 1 | 23.71 |
| 3.419 | 14 | 2 | 2 | 0 | 26.04 |
| 3.373M | 42 | 1 | 4 | 0 | 26.40 |
| 3.373M | | 1 | 3 | 1 | 26.40 |
| 3.111 | 2 | 2 | 1 | 1 | 28.67 |
| 2.831 | 7 | 0 | 0 | 2 | 31.58 |
| 2.685M | 41 | 2 | 4 | 0 | 33.35 |
| 2.685M | | 2 | 3 | 1 | 33.35 |
| 2.649 | 4 | 0 | 2 | 2 | 33.81 |
| 2.505 | 25 | 1 | 2 | 2 | 35.82 |
| 2.424 | 4 | 3 | 2 | 0 | 37.05 |
| 2.307 | 5 | 3 | 1 | 1 | 39.01 |
| 2.281 | 3 | 2 | 0 | 2 | 39.48 |
| 2.260 | 14 | 0 | 4 | 2 | 39.85 |
| 2.181 | 27 | 2 | 2 | 2 | 41.36 |
| 2.169 | 10 | 1 | 4 | 2 | 41.61 |
| 2.116M | 21 | 3 | 4 | 0 | 42.69 |
| 2.116M | | 3 | 3 | 1 | 42.69 |
| 2.097 | 3 | 2 | 6 | 0 | 43.11 |
| 2.005 | 1L | 0 | 7 | 1 | 45.18 |
| 1.9474 | 4 | 2 | 4 | 2 | 46.60 |
| 1.9415 | 2 | 1 | 7 | 1 | 46.75 |
| 1.9218 | 2 | 4 | 0 | 0 | 47.26 |
| 1.8733 | 5 | 0 | 1 | 3 | 48.56 |
| 1.8618 | 4 | 4 | 2 | 0 | 48.88 |
| 1.8424M | 13 | 3 | 5 | 1 | 49.43 |
| 1.8424M | | 3 | 2 | 2 | 49.43 |
| 1.8196 | 12 | 1 | 1 | 3 | 50.09 |
| 1.7896 | 3 | 3 | 6 | 0 | 50.99 |
| 1.7776 | 5 | 2 | 7 | 1 | 51.36 |
| 1.7215 | 2 | 1 | 3 | 3 | 53.16 |
| 1.7105M | 6 | 4 | 4 | 0 | 53.53 |
| 1.7105M | | 4 | 3 | 1 | 53.53 |
| 1.6852 | 14 | 2 | 6 | 2 | 54.40 |
| 1.5904 | 7 | 4 | 0 | 2 | 57.94 |
| 1.5650M | 6 | 1 | 5 | 3 | 58.97 |
| 1.5650M | | 0 | 8 | 2 | 58.97 |
| 1.5564M | 3 | 4 | 5 | 1 | 59.33 |
| 1.5564M | | 4 | 2 | 2 | 59.33 |

Aluminum Borate, $\text{Al}_{18}\text{B}_4\text{O}_{33}$ - (continued)

| $d(\text{\AA})$ | I^{rel} | hkl | $2\theta(^{\circ})$ |
|------------------|------------------|--------|---------------------|
| $\sigma = \pm 3$ | | | |
| 1.5330 | 2 | 1 8 2 | 60.33 |
| 1.5130M | 19 | 3 6 2 | 61.21 |
| 1.5130M | | 3 1 3 | 61.21 |
| 1.4764+ | 3 | 5 1 1 | 62.90 |
| 1.4764+ | | 2 5 3 | 62.90 |
| 1.4643 | 2 | 4 4 2 | 63.48 |
| 1.4496 | 7 | 2 8 2 | 64.20 |
| 1.4159 | 9 | 0 0 4 | 65.92 |
| 1.3982 | 2 | 2 10 0 | 66.86 |
| 1.3876 | 1 | 4 7 1 | 67.44 |
| 1.3694 | 2 | 1 2 4 | 68.46 |
| 1.3560 | 3 | 3 5 3 | 69.23 |
| 1.3425M | 3 | 4 8 0 | 70.03 |
| 1.3425M | | 4 6 2 | 70.03 |
| 1.3299+ | 10 | 5 2 2 | 70.79 |
| 1.3299+ | | 2 7 3 | 70.79 |
| 1.3067 | 6 | 1 10 2 | 72.24 |
| 1.2953 | 2 | 3 10 0 | 72.98 |
| 1.2810 | 1 | 6 0 0 | 73.93 |
| 1.2716 | 1 | 5 4 2 | 74.57 |
| 1.2631 | 1 | 6 2 0 | 75.16 |
| 1.2533M | 7 | 2 10 2 | 75.85 |
| 1.2533M | | 2 4 4 | 75.85 |
| 1.2513 | 6 | 0 12 0 | 75.99 |
| 1.2339 | 2 | 1 9 3 | 77.26 |
| 1.2296 | 1 | 4 9 1 | 77.58 |
| 1.2231 | 1 | 3 2 4 | 78.07 |
| 1.2129+ | 1 | 4 8 2 | 78.85 |
| 1.2129+ | | 6 4 0 | 78.85 |
| 1.1890+ | 1 | 5 6 2 | 80.76 |
| 1.1890+ | | 2 9 3 | 80.76 |
| 1.1770 | 2 | 3 4 4 | 81.76 |

Ammonium Borate Hydrate, $\text{NH}_4\text{B}_5\text{O}_8 \cdot 4\text{H}_2\text{O}$

Synonyms

1. Ammonium pentaborate tetrahydrate
2. APT

CAS registry no.
12229-12-8

Sample

The sample was obtained from Fisher Scientific Co., Fair Lawn, NJ. It was recrystallized from an aqueous solution at room temperature.

Color

Colorless

Structure

Orthorhombic, Bba2 (41), $Z = 4$ [Cook and Jaffe, 1957; Clark and Christ, 1959].

Lattice constants of this sample

$a = 11.033(3) \text{ \AA}$
 $b = 11.332(3)$
 $c = 9.238(3)$

$a/b = 0.9736$
 $c/b = 0.8152$

Volume

1155.0 \AA^3

Density

(calculated) 1.565 g/cm^3

Figure of merit

$F_{30} = 57.2 (0.014, 38)$

Reference intensity

$I/I_{\text{corundum}} = 1.08(6)$

Additional pattern

1. PDF card 12-638 [Clark and Christ, 1959]

References

- Clark, J. R. and Christ, C. L. (1959).
 Amer. Mineral. 44, 1150.
 Cook, W. R., Jr. and Jaffe, H. (1957).
 Acta Crystallogr. 10, 705.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$ | | | | |
|---|--------------------------------------|-----|---|---|
| Internal standard Si, $a = 5.43088 \text{ \AA}$ | | | | |
| $d(\text{Å})$ | I^{rel} $\sigma = \pm 2$ | hkl | | |
| 6.00 | 63 | 1 | 1 | 1 |
| 5.67 | 12 | 0 | 2 | 0 |
| 5.52 | 46 | 2 | 0 | 0 |
| 4.951 | 2 | 2 | 1 | 0 |
| 4.617 | 7 | 0 | 0 | 2 |
| 4.427 | 1 | 1 | 2 | 1 |
| 3.544 | 80 | 2 | 0 | 2 |
| 3.383 | 100 | 2 | 1 | 2 |
| 3.334 | 11 | 1 | 3 | 1 |
| 3.271 | 9 | 3 | 1 | 1 |
| 3.003 | 4 | 2 | 2 | 2 |
| 2.926 | 7 | 3 | 2 | 1 |
| 2.868 | 4 | 1 | 1 | 3 |
| 2.834 | 31 | 0 | 4 | 0 |
| 2.760 | 2 | 4 | 0 | 0 |
| 2.680 | 2 | 4 | 1 | 0 |
| 2.627 | 5 | 1 | 2 | 3 |
| 2.586 | 1 | 2 | 3 | 2 |
| 2.533 | 8 | 3 | 3 | 1 |
| 2.479 | 1L | 4 | 2 | 0 |
| 2.414 | 1 | 0 | 4 | 2 |
| 2.367 | 4 | 4 | 0 | 2 |
| 2.332 | 4 | 1 | 3 | 3 |
| 2.317 | 9 | 4 | 1 | 2 |
| 2.312M | 9 | 3 | 1 | 3 |
| 2.312M | | 0 | 0 | 4 |
| 2.212 | 8 | 2 | 4 | 2 |
| 2.182 | 16 | 3 | 4 | 1 |
| 2.178 | 16 | 3 | 2 | 3 |
| 2.158 | 4 | 1 | 5 | 1 |
| 2.138 | 3 | 0 | 2 | 4 |
| 2.107 | 7 | 5 | 1 | 1 |
| 2.095M | 2 | 2 | 5 | 0 |
| 2.095M | | 2 | 1 | 4 |
| 2.048 | 2 | 1 | 4 | 3 |
| 2.007M | 7 | 5 | 2 | 1 |
| 2.007M | | 4 | 3 | 2 |
| 1.909 | 6 | 2 | 5 | 2 |
| 1.888M | 2 | 3 | 5 | 1 |
| 1.888M | | 0 | 6 | 0 |
| 1.856 | 4 | 2 | 3 | 4 |
| 1.817 | 4 | 4 | 4 | 2 |
| 1.7998M | 2 | 1 | 5 | 3 |
| 1.7998M | | 1 | 1 | 5 |
| 1.7715M | 3 | 5 | 1 | 3 |

Ammonium Borate Hydrate, $\text{NH}_4\text{B}_5\text{O}_8 \cdot 4\text{H}_2\text{O}$ - (continued)

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 2$ | hkl | $2\theta(^{\circ})$ |
|-----------------|--------------------------------------|-------|---------------------|
| 1.7715M | | 4 0 4 | 51.55 |
| 1.7506M | 3 | 4 5 0 | 52.21 |
| 1.7506M | | 4 1 4 | 52.21 |
| 1.7102M | 2 | 5 4 1 | 53.54 |
| 1.7102M | | 5 2 3 | 53.54 |
| 1.7029 | 2 | 2 4 4 | 53.79 |
| 1.6533M | 1 | 6 3 0 | 55.54 |
| 1.6533M | | 3 6 1 | 55.54 |
| 1.6206 | 1L | 5 3 3 | 56.76 |
| 1.5780 | 1 | 1 7 1 | 58.44 |
| 1.5427 | 1 | 6 4 0 | 59.91 |

Ammonium Nickel Sulfate Hydrate, $(\text{NH}_4)_2\text{Ni}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$

CAS registry no.
51287-85-5

Sample

The sample was obtained from the Fisher Scientific Co., Fair Lawn, NJ.

Color

Strong bluish green

Structure

Monoclinic, $P2_1/a$ (14), $Z = 2$. The structure was determined by Grimes et al. [1963] and by Montgomery and Lingafelter [1964]. It is isostructural with other "Tutton" salts [Tutton, 1916].

Lattice constants of this sample

$a = 9.1862(15) \text{ \AA}$
 $b = 12.468(2)$
 $c = 6.2423(10)$
 $\beta = 106.93(2)^\circ$

$a/b = 0.7368$
 $c/b = 0.5007$

Volume $^\circ$
 684.0 \AA^3

Density

(calculated) 1.918 g/cm^3

Figure of merit

$F_{30} = 63.7(0.012, 38)$

Reference intensity

$I/I_{\text{corundum}} = 0.92(5)$

Additional pattern

1. PDF card 12-454 [Institute of Physics, Cardiff, Wales]

References

Grimes, N. W., Kay, H. F., and Webb, M. W. (1963). *Acta Crystallogr.* **16**, 823.
Montgomery, H. and Lingafelter, E. C. (1964). *Acta Crystallogr.* **17**, 1478.
Tutton, A. E. (1916). *Trans. Roy. Soc. London Ser. A* **216**, 1.

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 5$ | hkl | $2\theta(^\circ)$ |
|-----------------|--------------------------------------|--------|-------------------|
| 5.090 | 20 | 1 2 0 | 17.41 |
| 4.397 | 19 | 2 0 0 | 20.18 |
| 4.316 | 21 | 0 2 1 | 20.56 |
| 4.243 | 36 | -1 2 1 | 20.92 |
| 4.166 | 100 | -2 0 1 | 21.31 |
| 4.147 | 66 | 2 1 0 | 21.41 |
| 3.952 | 6 | -2 1 1 | 22.48 |
| 3.757 | 88 | 1 3 0 | 23.66 |
| 3.586 | 16 | 1 2 1 | 24.81 |
| 3.466 | 4 | -2 2 1 | 25.68 |
| 3.410 | 14 | 0 3 1 | 26.11 |
| 3.376 | 18 | -1 3 1 | 26.38 |
| 3.119 | 20 | 0 4 0 | 28.60 |
| 3.037 | 32 | 2 1 1 | 29.39 |
| 3.027 | 44 | -1 1 2 | 29.49 |
| 2.943 | 4 | -2 3 1 | 30.35 |
| 2.913 | 4 | -3 1 1 | 30.67 |
| 2.903 | 5 | 0 1 2 | 30.77 |
| 2.892 | 6 | -2 0 2 | 30.89 |
| 2.853 | 6 | 3 1 0 | 31.33 |
| 2.816 | 6 | -2 1 2 | 31.75 |
| 2.796 | 28 | 2 2 1 | 31.98 |
| 2.790 | 26 | -1 2 2 | 32.05 |
| 2.742 | 3 | -1 4 1 | 32.63 |
| 2.703 | 8 | -3 2 1 | 33.12 |
| 2.651 | 1 | 3 2 0 | 33.79 |
| 2.623 | 2 | -2 2 2 | 34.16 |
| 2.550 | 6 | 1 1 2 | 35.17 |
| 2.541M | 11 | 2 4 0 | 35.29 |
| 2.541M | | 1 4 1 | 35.29 |
| 2.501 | 7 | 2 3 1 | 35.88 |
| 2.430 | 25 | -3 3 1 | 36.96 |
| 2.395 | 3 | 3 3 0 | 37.52 |
| 2.374 | 2 | -2 3 2 | 37.86 |
| 2.302 | 2 | 0 5 1 | 39.10 |
| 2.208M | 16 | 1 3 2 | 40.84 |
| 2.208M | | 2 4 1 | 40.84 |
| 2.166+ | 7 | 1 5 1 | 41.67 |
| 2.166+ | | 4 1 0 | 41.67 |
| 2.156M | 9 | 0 4 2 | 41.86 |
| 2.156M | | 2 1 2 | 41.86 |
| 2.134 | 9 | 3 4 0 | 42.31 |
| 2.120 | 6 | -2 4 2 | 42.62 |
| 2.072 | 10 | 4 2 0 | 43.64 |
| 2.052 | 2 | -2 0 3 | 44.09 |
| 2.049 | 2 | -1 1 3 | 44.17 |
| 2.024 | 3 | -2 1 3 | 44.74 |
| 2.005 | 1 | -4 3 1 | 45.19 |
| 1.990 | 4 | 0 0 3 | 45.54 |
| 1.975 | 2 | -4 2 2 | 45.92 |
| 1.963 | 4 | 0 6 1 | 46.22 |
| 1.956 | 3 | -1 6 1 | 46.39 |
| 1.950M | 2 | 2 5 1 | 46.53 |
| 1.950M | | -2 2 3 | 46.53 |
| 1.942M | 2 | 4 3 0 | 46.73 |

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}; \text{ temp. } 25 \pm 1^\circ \text{C}$ | | | |
|---|--------------------------------------|--------|-------------------|
| Internal standard W, $a = 3.16524 \text{ \AA}$ | | | |
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 5$ | hkl | $2\theta(^\circ)$ |
| 7.19 | 4 | 1 1 0 | 12.30 |
| 6.24 | 30 | 0 2 0 | 14.19 |
| 5.98 | 14 | 0 0 1 | 14.80 |
| 5.388 | 36 | 0 1 1 | 16.44 |
| 5.248 | 7 | -1 1 1 | 16.88 |

Ammonium Nickel Sulfate Hydrate, $(\text{NH}_4)_2\text{Ni}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ - (continued)

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 5$ | hkl | $2\theta(^{\circ})$ |
|-----------------|--------------------------------------|--------|---------------------|
| 1.942M | | -3 4 2 | 46.73 |
| 1.915 | 7 | 0 5 2 | 47.43 |
| 1.905 | 10 | -3 1 3 | 47.71 |
| 1.899 | 10 | 3 5 0 | 47.87 |
| 1.878M | 3 | 1 6 1 | 48.44 |
| 1.878M | | 2 6 0 | 48.44 |
| 1.8575 | 7 | -1 3 3 | 49.00 |
| 1.8389 | 6 | -2 3 3 | 49.53 |
| 1.8179 | 3 | -5 1 1 | 50.14 |
| 1.8095M | 5 | 4 2 1 | 50.39 |
| 1.8095M | | 1 1 3 | 50.39 |
| 1.7949M | 10 | 0 3 3 | 50.83 |
| 1.7949M | | 4 4 0 | 50.83 |
| 1.7919 | 8 | 2 4 2 | 50.92 |
| 1.7632 | 2 | -5 2 1 | 51.81 |
| 1.7588 | 4 | -3 5 2 | 51.95 |
| 1.7401 | 4 | 5 1 0 | 52.55 |
| 1.7288M | 2 | -1 6 2 | 52.92 |
| 1.7288M | | -1 4 3 | 52.92 |
| 1.7176 | 5 | 3 5 1 | 53.29 |
| 1.7132 | 6 | -2 4 3 | 53.44 |
| 1.7052 | 2 | 0 6 2 | 53.71 |
| 1.6855M | 5 | -4 2 3 | 54.39 |
| 1.6855M | | -4 5 1 | 54.39 |
| 1.6826 | 4 | 3 3 2 | 54.49 |
| 1.6750 | 3 | 1 3 3 | 54.76 |

Ammonium Sulfate, (NH₄)₂S₂O₃

Synonym

1. Ammonium thiosulfate

CAS registry no.

7783-18-8

Sample

The sample was obtained from the Fisher Scientific Co., Fair Lawn, NJ.

Color

Colorless

Structure

Monoclinic, C2/m (12), Z = 4. The structure was determined by Brunt [1946]. A line at 2θ = 23.06 with I = 4, could not be indexed.

Lattice constants of this sample

a = 10.2233(15) Å

b = 6.4956(9)

c = 8.8074(10)

β = 94.66(1)°

a/b = 1.5739

c/b = 1.3559

Volume

582.93 Å³

Density

(calculated) 1.689 g/cm³

Figure of merit

F₃₀ = 91.0(0.010,34)

Reference intensity

I/I_{corundum} = 0.94(3)

Additional pattern

1. PDF card 1-844 [Hanawalt et al., 1938]

References

Brunt, N. A. (1946). Diss. Leiden pp. 64.

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C | | | | |
|---|----------------------------|--------|-------|--|
| Internal standard Si, a = 5.43088 Å | | | | |
| d(Å) | I ^{rel} σ = ±8 | hkl | 2θ(°) | |
| 5.480 | 16 | 1 1 0 | 16.16 | |
| 5.093 | 44 | 2 0 0 | 17.40 | |
| 4.741 | 93 | -1 1 1 | 18.70 | |
| 4.553 | 100 | 1 1 1 | 19.48 | |
| 4.386 | 76 | 0 0 2 | 20.23 | |

| d(Å) | I ^{rel} σ = ±8 | hkl | 2θ(°) |
|---------|----------------------------|--------|-------|
| 4.257 | 18 | 2 0 1 | 20.85 |
| 3.501 | 16 | -1 1 2 | 25.42 |
| 3.469 | 14 | -2 0 2 | 25.66 |
| 3.353 | 32 | 1 1 2 | 26.56 |
| 3.248 | 18 | 0 2 0 | 27.44 |
| 3.199 | 28 | 2 0 2 | 27.87 |
| 3.046 | 22 | 0 2 1 | 29.30 |
| 3.010 | 74 | 3 1 0 | 29.66 |
| 2.925 | 8 | 0 0 3 | 30.54 |
| 2.915 | 9 | -3 1 1 | 30.65 |
| 2.785 | 9 | 3 1 1 | 32.11 |
| 2.739 | 6 | 2 2 0 | 32.67 |
| 2.629M | 62 | -2 0 3 | 34.07 |
| 2.629M | | -1 1 3 | 34.07 |
| 2.612 | 32 | 0 2 2 | 34.31 |
| 2.582 | 14 | 2 2 1 | 34.71 |
| 2.569 | 13 | -3 1 2 | 34.90 |
| 2.547 | 8 | 4 0 0 | 35.21 |
| 2.536 | 8 | 1 1 3 | 35.36 |
| 2.500 | 2 | -4 0 1 | 35.89 |
| 2.453 | 5 | 2 0 3 | 36.61 |
| 2.402 | 6 | 3 1 2 | 37.41 |
| 2.395 | 6 | 4 0 1 | 37.52 |
| 2.371 | 20 | -2 2 2 | 37.92 |
| 2.286 | 6 | -4 0 2 | 39.39 |
| 2.280 | 6 | 2 2 2 | 39.50 |
| 2.195 | 6 | 0 0 4 | 41.09 |
| 2.178 | 6 | -3 1 3 | 41.42 |
| 2.129 | 3 | 4 0 2 | 42.42 |
| 2.118 | 2 | 1 3 0 | 42.65 |
| 2.078 | 4 | -2 0 4 | 43.51 |
| 2.0688M | 5 | -1 1 4 | 43.72 |
| 2.0688M | | -1 3 1 | 43.72 |
| 2.0510 | 4 | 1 3 1 | 44.12 |
| 2.0444 | 4 | -2 2 3 | 44.27 |
| 2.0270 | 2 | 3 1 3 | 44.67 |
| 2.0065 | 6 | 1 1 4 | 45.15 |
| 1.9824 | 2 | -4 2 1 | 45.73 |
| 1.9582M | 7 | 2 0 4 | 46.33 |
| 1.9582M | | 2 2 3 | 46.33 |
| 1.9451 | 3 | 5 1 0 | 46.66 |
| 1.9271 | 3 | 4 2 1 | 47.12 |
| 1.8946 | 3 | 1 3 2 | 47.98 |
| 1.8686M | 3 | -4 2 2 | 48.69 |
| 1.8686M | | 5 1 1 | 48.69 |
| 1.8368 | 2 | -3 1 4 | 49.59 |
| 1.8319 | 2 | -5 1 2 | 49.73 |
| 1.8261 | 4 | 3 3 0 | 49.90 |
| 1.8186 | 12 | 0 2 4 | 50.12 |
| 1.8031 | 7 | -3 3 1 | 50.58 |

Ammonium Sulfate, $(\text{NH}_4)_2\text{S}_2\text{O}_3$ - (continued)

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 8$ | hkl | $2\theta(^{\circ})$ |
|-----------------|--------------------------------------|--------|---------------------|
| 1.7814 | 2 | 4 2 2 | 51.24 |
| 1.7559 | 5 | 0 0 5 | 52.04 |
| 1.7294M | 10 | -1 3 3 | 52.90 |
| 1.7294M | | 5 1 2 | 52.90 |
| 1.7159 | 3 | 3 1 4 | 53.35 |
| 1.7117 | 4 | -3 3 2 | 53.49 |
| 1.7052 | 6 | -4 2 3 | 53.71 |
| 1.7023M | 6 | -2 0 5 | 53.81 |
| 1.7023M | | 1 3 3 | 53.81 |
| 1.6933M | 6 | -1 1 5 | 54.12 |
| 1.6933M | | -6 0 1 | 54.12 |
| 1.6801 | 4 | -5 1 3 | 54.58 |
| 1.6775 | 4 | 2 2 4 | 54.67 |
| 1.6599 | 2 | 3 3 2 | 55.30 |
| 1.6508 | 2 | 1 1 5 | 55.63 |
| 1.6196 | 1 | 2 0 5 | 56.80 |
| 1.6066 | 1 | 4 2 3 | 57.30 |
| 1.5967 | 1 | 0 4 1 | 57.69 |
| 1.5809 | 2 | -3 3 3 | 58.32 |
| 1.5665 | 4 | -3 1 5 | 58.91 |

Ammonium Sulfate, $(\text{NH}_4)_2\text{S}_2\text{O}_8$

Synonym
Ammonium persulfate

Sample
The sample was from Fisher Scientific Co.
Fair Lawn, NJ. The sample was hygroscopic.

Color
Colorless

Structure
Monoclinic, $\text{P2}_1/\text{n}(14)$, $Z = 2$. The structure of $(\text{NH}_4)_2\text{S}_2\text{O}_8$ has been determined by Zachariasen and Mooney [1934] and refined by Sivertsen and Sorum [1969].

Lattice constants of this sample

$a = 7.829(2)$
 $b = 8.0075(14)$
 $c = 6.1483(12)$
 $\beta = 95.12(2)^\circ$

$a/b = 0.9777$
 $c/b = 0.7678$

Volume
 383.90 \AA^3

Density
(calculated) 1.974 g/cm^3

Figure of merit
 $F_{30} = 41.9(0.015, 48)$

Additional pattern
1. PDF card 11-551 [University College, Cardiff, Wales]

References
Sivertsen, B. K. and Sorum, H. (1969) Z.
Kristallogr. Kristallgeometrie Kristallphys.
Kristallchem. 130, 449.
Zachariasen, W. H. and Mooney, R. C. L. (1934)
Z. Kristallogr. Kristallgeometrie Kristallphys.
Kristallchem. 88, 63.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$ | | | |
|---|--------------------------------------|--------|-------------------|
| Internal standard W, $a = 3.16524 \text{ \AA}$ | | | |
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 6$ | hkl | $2\theta(^\circ)$ |
| 5.583 | 42 | 1 1 0 | 15.86 |
| 5.038 | 62 | -1 0 1 | 17.59 |
| 4.862 | 14 | 0 1 1 | 18.23 |
| 4.621 | 10 | 1 0 1 | 19.19 |
| 4.261 | 12 | -1 1 1 | 20.83 |

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 6$ | hkl | $2\theta(^\circ)$ |
|-----------------|--------------------------------------|--------|-------------------|
| 3.996M | 50 | 0 2 0 | 22.23 |
| 3.996M | | 1 1 1 | 22.23 |
| 3.560 | 62 | 1 2 0 | 24.99 |
| 3.501 | 69 | 2 1 0 | 25.42 |
| 3.347 | 100 | 0 2 1 | 26.61 |
| 3.154 | 50 | -2 1 1 | 28.27 |
| 3.063 | 16 | 0 0 2 | 29.13 |
| 3.027 | 2 | 1 2 1 | 29.49 |
| 2.945 | 19 | 2 1 1 | 30.33 |
| 2.860 | 18 | 0 1 2 | 31.25 |
| 2.761 | 2 | -1 1 2 | 32.40 |
| 2.606 | 6 | -2 2 1 | 34.39 |
| 2.526 | 3 | 1 3 0 | 35.51 |
| 2.483 | 28 | 2 2 1 | 36.15 |
| 2.475M | 25 | -3 0 1 | 36.27 |
| 2.475M | | 3 1 0 | 36.27 |
| 2.433 | 6 | 0 2 2 | 36.92 |
| 2.403 | 13 | -2 1 2 | 37.39 |
| 2.370 | 4 | -1 2 2 | 37.93 |
| 2.309M | 8 | 1 3 1 | 38.97 |
| 2.309M | | 2 0 2 | 38.97 |
| 2.220 | 10 | 2 1 2 | 40.61 |
| 2.204 | 8 | 2 3 0 | 40.92 |
| 2.181 | 2 | 3 2 0 | 41.36 |
| 2.041 | 16 | 2 3 1 | 44.35 |
| 2.019 | 2 | -1 0 3 | 44.85 |
| 2.012 | 4 | 0 3 2 | 45.01 |
| 2.007 | 6 | 3 2 1 | 45.14 |
| 1.978M | 5 | 0 1 3 | 45.84 |
| 1.978M | | -1 3 2 | 45.84 |
| 1.940 | 3 | 1 4 0 | 46.80 |
| 1.933 | 8 | 1 0 3 | 46.97 |
| 1.921 | 4 | 1 3 2 | 47.27 |
| 1.8791 | 4 | 1 1 3 | 48.40 |
| 1.8625 | 6 | 3 3 0 | 48.86 |
| 1.8424 | 2 | -3 2 2 | 49.43 |
| 1.8368 | 6 | 1 4 1 | 49.59 |
| 1.8145 | 2 | -3 3 1 | 50.24 |
| 1.7805 | 8 | 2 4 0 | 51.27 |
| 1.7660 | 2 | 4 1 1 | 51.72 |
| 1.7509 | 3 | 3 3 1 | 52.20 |
| 1.7459 | 3 | 2 3 2 | 52.36 |
| 1.7285 | 2 | -2 4 1 | 52.93 |
| 1.7221 | 11 | -4 2 1 | 53.14 |
| 1.6750 | 2 | 0 4 2 | 54.76 |
| 1.6549 | 2 | -1 4 2 | 55.48 |
| 1.6505 | 4 | 4 2 1 | 55.64 |
| 1.6000 | 3 | 2 2 3 | 57.56 |

Cadmium Bromate Hydrate, $\text{Cd}(\text{BrO}_3)_2 \cdot 2\text{H}_2\text{O}$

Synonym

1. Cadmium bromate dihydrate

CAS registry no.

19320-65-1

Sample

The sample was prepared by dissolving anhydrous $\text{Cd}(\text{BrO}_3)_2$ in water and letting it dry. The sample was then washed.

Color

Light orange yellow.

Structure

Orthorhombic, $P2_12_12_1$ (19), $Z = 4$. The structure was studied by Garcia-Blanco and Perales [1963].

Lattice constants of this sample

$a = 9.2417(10) \text{ \AA}$

$b = 12.5015(13)$

$c = 6.1762(6)$

$a/b = 0.7392$

$c/b = 0.4940$

Volume

713.57 \AA^3

Density

(calculated) 3.763 g/cm^3

Figure of merit

$F_{30} = 62.5(0.012, 39)$

Reference intensity

$I/I_{\text{corundum}} = 2.9(2)$

Additional pattern

1. PDF card 1-0353 (labelled monohydrate) [Hanawalt et al. 1938]

References

Garcia-Blanco, S. and Perales, A. (1963). Acta Crystallogr. 16, A34.

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$ | | | |
|---|--------------------------------------|-------|-------------------|
| Internal standard W, $a = 3.16524 \text{ \AA}$ | | | |
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 1$ | hkl | $2\theta(^\circ)$ |
| 6.24 | 22 | 0 2 0 | 14.18 |
| 5.538 | 28 | 0 1 1 | 15.99 |
| 5.172 | 1 | 1 2 0 | 17.13 |
| 5.131 | 1 | 1 0 1 | 17.27 |
| 4.746 | 4 | 1 1 1 | 18.68 |
| 4.621 | 1 | 2 0 0 | 19.19 |
| 4.397 | 100 | 0 2 1 | 20.18 |
| 3.969 | 4 | 1 2 1 | 22.38 |
| 3.799 | 2 | 1 3 0 | 23.40 |
| 3.714 | 15 | 2 2 0 | 23.94 |
| 3.700 | 15 | 2 0 1 | 24.03 |
| 3.546 | 21 | 2 1 1 | 25.09 |
| 3.453 | 22 | 0 3 1 | 25.78 |
| 3.236 | 11 | 1 3 1 | 27.54 |
| 3.184 | 26 | 2 2 1 | 28.00 |
| 3.123 | 12 | 0 4 0 | 28.56 |
| 3.091M | 24 | 2 3 0 | 28.86 |
| 3.091M | | 0 0 2 | 28.86 |
| 2.996 | 5 | 0 1 2 | 29.80 |
| 2.990 | 5 | 3 1 0 | 29.86 |
| 2.959 | 3 | 1 4 0 | 30.18 |
| 2.929 | 1L | 1 0 2 | 30.50 |
| 2.851 | 14 | 1 1 2 | 31.35 |
| 2.769M | 16 | 0 2 2 | 32.31 |
| 2.769M | | 2 3 1 | 32.31 |
| 2.692 | 5 | 3 1 1 | 33.25 |
| 2.669 | 3 | 1 4 1 | 33.55 |
| 2.651 | 3 | 1 2 2 | 33.79 |
| 2.590 | 3 | 2 4 0 | 34.61 |
| 2.568 | 2 | 2 0 2 | 34.91 |
| 2.514 | 10 | 2 1 2 | 35.68 |
| 2.480 | 4 | 0 3 2 | 36.19 |
| 2.477 | 3 | 3 3 0 | 36.24 |
| 2.396 | 5 | 1 3 2 | 37.51 |
| 2.389 | 6 | 2 4 1 | 37.62 |
| 2.375 | 7 | 2 2 2 | 37.85 |
| 2.318 | 5 | 0 5 1 | 38.81 |
| 2.273 | 8 | 4 1 0 | 39.62 |
| 2.248 | 5 | 1 5 1 | 40.07 |
| 2.196M | 22 | 0 4 2 | 41.07 |
| 2.196M | | 3 4 0 | 41.07 |
| 2.181 | 5 | 3 0 2 | 41.36 |
| 2.164 | 2 | 4 0 1 | 41.70 |
| 2.148 | 3 | 3 1 2 | 42.02 |
| 2.137 | 6 | 1 4 2 | 42.25 |

Cadmium Bromate Hydrate, $\text{Cd}(\text{BrO}_3)_2 \cdot 2\text{H}_2\text{O}$ - (continued)

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 1$ | hkl | $2\theta(^{\circ})$ |
|-----------------|--------------------------------------|-------|---------------------|
| 2.133 | 5 | 4 1 1 | 42.35 |
| 2.083 | 4 | 0 6 0 | 43.41 |
| 2.071 | 11 | 2 5 1 | 43.68 |
| 2.067 | 10 | 3 4 1 | 43.77 |
| 2.044 | 5 | 4 2 1 | 44.27 |
| 2.033M | 9 | 1 6 0 | 44.54 |
| 2.033M | | 0 1 3 | 44.54 |
| 2.011 | 3 | 1 0 3 | 45.05 |
| 1.9845M | 4 | 1 1 3 | 45.68 |
| 1.9845M | | 2 4 2 | 45.68 |
| 1.9747 | 2 | 0 6 1 | 45.92 |
| 1.9443 | 10 | 0 5 2 | 46.68 |
| 1.9322M | 3 | 3 3 2 | 46.99 |
| 1.9322M | | 1 6 1 | 46.99 |
| 1.9195 | 4 | 4 3 1 | 47.32 |
| 1.9122 | 5 | 1 2 3 | 47.51 |
| 1.9013 | 1 | 1 5 2 | 47.80 |
| 1.8810 | 1 | 2 0 3 | 48.35 |
| 1.8597 | 1 | 2 1 3 | 48.94 |
| 1.8501 | 2 | 4 0 2 | 49.21 |
| 1.8462 | 1 | 0 3 3 | 49.32 |
| 1.8285 | 1 | 5 1 0 | 49.83 |
| 1.8159 | 5 | 2 6 1 | 50.20 |
| 1.8008 | 3 | 2 2 3 | 50.65 |
| 1.7886 | 4 | 3 4 2 | 51.02 |
| 1.7789 | 3 | 4 4 1 | 51.32 |
| 1.7547M | 1 | 1 7 0 | 52.08 |
| 1.7547M | | 5 1 1 | 52.08 |
| 1.7194 | 2 | 0 4 3 | 53.23 |
| 1.7147M | 4 | 0 7 1 | 53.39 |
| 1.7147M | | 2 3 3 | 53.39 |
| 1.7040 | 2 | 5 2 1 | 53.75 |
| 1.6967+ | 3 | 4 5 0 | 54.00 |
| 1.6967+ | | 3 1 3 | 54.00 |
| 1.6904+ | 6 | 1 4 3 | 54.22 |
| 1.6904+ | | 5 3 0 | 54.22 |
| 1.6872 | 5 | 1 7 1 | 54.33 |
| 1.6665 | 2 | 2 7 0 | 55.06 |
| 1.6621 | 3 | 3 6 1 | 55.22 |
| 1.6511 | 1 | 3 2 3 | 55.62 |
| 1.6432 | 3 | 3 5 2 | 55.91 |
| 1.6362 | 2 | 4 5 1 | 56.17 |
| 1.6298 | 3 | 5 3 1 | 56.41 |
| 1.6177 | 1 | 2 6 2 | 56.87 |
| 1.6110 | 3 | 2 4 3 | 57.13 |

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 1$ | hkl | $2\theta(^{\circ})$ |
|-----------------|--------------------------------------|-------|---------------------|
| 1.6084 | 3 | 2 7 1 | 57.23 |
| 1.5921 | 2 | 4 4 2 | 57.87 |
| 1.5901M | 2 | 5 4 0 | 57.95 |
| 1.5901M | | 0 5 3 | 57.95 |
| 1.5831 | 4 | 3 3 3 | 58.23 |
| 1.5735 | 1 | 5 1 2 | 58.62 |
| 1.5633 | 2 | 0 8 0 | 59.04 |
| 1.5457M | 2 | 0 7 2 | 59.78 |
| 1.5457M | | 3 7 0 | 59.78 |
| 1.5413M | 3 | 1 8 0 | 59.97 |
| 1.5413M | | 5 4 1 | 59.97 |
| 1.5373M | 2 | 5 2 2 | 60.14 |
| 1.5373M | | 4 0 3 | 60.14 |
| 1.5327 | 3 | 0 1 4 | 60.34 |
| 1.5243 | 1 | 1 7 2 | 60.71 |
| 1.5146 | 2 | 0 8 1 | 61.14 |
| 1.5117 | 3 | 1 1 4 | 61.27 |
| 1.5030 | 1 | 2 5 3 | 61.66 |
| 1.5006M | 1 | 3 4 3 | 61.77 |
| 1.5006M | | 4 6 1 | 61.77 |
| 1.4989M | 1 | 0 2 4 | 61.85 |
| 1.4989M | | 3 7 1 | 61.85 |
| 1.4945M | 1 | 1 8 1 | 62.05 |
| 1.4945M | | 6 0 1 | 62.05 |
| 1.4866M | 2 | 4 5 2 | 62.42 |
| 1.4866M | | 5 5 0 | 62.42 |
| 1.4838 | 3 | 6 1 1 | 62.55 |
| 1.4657 | 3 | 2 7 2 | 63.41 |
| 1.4641M | 3 | 2 0 4 | 63.49 |
| 1.4641M | | 0 6 3 | 63.49 |
| 1.4482 | 3 | 0 3 4 | 64.27 |
| 1.4445M | 2 | 5 5 1 | 64.45 |
| 1.4445M | | 6 3 0 | 64.45 |
| 1.4303 | 2 | 1 3 4 | 65.17 |
| 1.4255 | 1 | 2 2 4 | 65.42 |
| 1.4130M | 1 | 4 7 0 | 66.07 |
| 1.4130M | | 3 5 3 | 66.07 |
| 1.4070 | 1 | 6 3 1 | 66.39 |
| 1.3942M | 2 | 0 8 2 | 67.08 |
| 1.3942M | | 3 8 0 | 67.08 |

Calcium Sulfate Hydrate (Gypsum), $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$

Synonym

1. Calcium sulfate dihydrate

CAS registry no.

10101-41-4

Sample

The sample was prepared by adding H_2SO_4 to a water solution of $\text{Ca}(\text{NO}_3)_2$. The precipitate was filtered out, washed in water, and bottled while moist. The crystals were dried immediately before use, and care was taken to prevent dehydration.

Color

Colorless

Structure

Monoclinic, C2/c (15), $Z = 4$. The structure was determined by Wooster [1936] and refined by Atoji and Rundle [1958].

Lattice constants of this sample

$a = 6.2845(11) \text{ \AA}$

$b = 15.2079(15)$

$c = 5.6776(7)$

$\beta = 114.09(1)^\circ$

$a/b = 0.4132$

$c/b = 0.3733$

Volume

495.37 \AA^3

Density

(calculated) 2.308 g/cm^3

Figure of merit

$F_{30} = 47.4(0.013, 49)$

Reference intensity

$I/I_{\text{corundum}} = 1.83(4)$

Additional patterns

1. PDF card 6-0046 [F. H. Gillery, Pennsylvania State University, University Park, PA]

2. PDF card 21-816 [Technisch Physische Dienst, Delft, Holland]

References

Atoji, M. and Rundle, R. E. (1958). J. Chem. Phys. **29**, 1306.

Wooster, W. A. (1936). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. **94**, 375.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$ Internal standard Si, $a = 5.43088 \text{ \AA}$ | | | |
|--|--------------------------------------|--------|-------------------|
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 4$ | hkl | $2\theta(^\circ)$ |
| 7.63 | 100 | 0 2 0 | 11.59 |
| 4.283 | 98 | 0 2 1 | 20.72 |
| 3.799M | 17 | 0 4 0 | 23.40 |
| 3.799M | | 1 3 0 | 23.40 |
| 3.172 | 4 | 1 1 1 | 28.11 |
| 3.065 | 74 | 0 4 1 | 29.11 |
| 2.873 | 47 | -2 2 1 | 31.10 |
| 2.789 | 10 | -1 1 2 | 32.07 |
| 2.732 | 2 | 1 3 1 | 32.75 |
| 2.685M | 34 | 1 5 0 | 33.35 |
| 2.685M | | 2 2 0 | 33.35 |
| 2.597 | 6 | -1 5 1 | 34.51 |
| 2.534 | 2 | 0 6 0 | 35.39 |
| 2.495 | 11 | -2 0 2 | 35.97 |
| 2.476 | 1 | -1 3 2 | 36.25 |
| 2.452 | 6 | 0 2 2 | 36.62 |
| 2.406 | 4 | -2 4 1 | 37.35 |
| 2.291 | 1L | 2 4 0 | 39.29 |
| 2.219 | 15 | 1 5 1 | 40.63 |
| 2.142 | 2 | 0 4 2 | 42.15 |
| 2.086 | 24 | -2 4 2 | 43.34 |
| 2.074M | 15 | -1 5 2 | 43.60 |
| 2.074M | | -3 1 1 | 43.60 |
| 2.048 | 6 | 1 1 2 | 44.18 |
| 2.032 | 1L | 1 7 0 | 44.56 |
| 1.992 | 4 | -1 7 1 | 45.51 |
| 1.963 | 3 | -2 6 1 | 46.22 |
| 1.8998M | 16 | 0 8 0 | 47.84 |
| 1.8998M | | 2 6 0 | 47.84 |
| 1.8795 | 12 | 2 4 1 | 48.39 |
| 1.8650 | 3 | -1 1 3 | 48.79 |
| 1.8118 | 13 | 0 6 2 | 50.32 |
| 1.7995 | 6 | -2 2 3 | 50.69 |
| 1.7844 | 9 | 0 8 1 | 51.15 |
| 1.7785 | 12 | -2 6 2 | 51.33 |
| 1.7093 | 1 | 1 5 2 | 53.57 |
| 1.6846 | 3 | 0 2 3 | 54.42 |
| 1.6640 | 6 | -2 4 3 | 55.15 |
| 1.6456 | 4 | 2 6 1 | 55.82 |
| 1.6209+ | 9 | -2 8 1 | 56.75 |
| 1.6209+ | | 1 9 0 | 56.75 |
| 1.6005 | 1 | -1 9 1 | 57.54 |
| 1.5846 | 4 | 2 8 0 | 58.17 |
| 1.5327 | 2 | 0 8 2 | 60.34 |
| 1.5209+ | 1 | 0 10 0 | 60.86 |

Calcium Sulfate Hydrate (Gypsum), $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$ - (continued)

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 4$ | hkl | $2\theta(^{\circ})$ |
|-----------------|--------------------------------------|---------|---------------------|
| 1.5209+ | | -4 2 2 | 60.86 |
| 1.5119 | 1 | -2 8 2 | 61.26 |
| 1.4982 | 1L | 1 9 1 | 61.88 |
| 1.4947 | 1L | -2 6 3 | 62.04 |
| 1.4591+ | 3 | -3 7 2 | 63.73 |
| 1.4591+ | | 0 10 1 | 63.73 |
| 1.4392 | 5 | -4 4 1 | 64.72 |
| 1.4354 | 3 | 3 7 0 | 64.91 |
| 1.4278M | 2 | 2 8 1 | 65.30 |
| 1.4278M | | 0 6 3 | 65.30 |
| 1.4178 | 3 | -2 0 4 | 65.82 |
| 1.4015 | 2 | -4 2 3 | 66.68 |
| 1.3657M | 5 | 2 6 2 | 68.67 |
| 1.3657M | | -2 10 1 | 68.67 |
| 1.3440M | 1 | 1 11 0 | 69.94 |
| 1.3440M | | 2 10 0 | 69.94 |
| 1.3324 | 2 | -1 11 1 | 70.64 |
| 1.3262 | 4 | -2 8 3 | 71.02 |
| 1.3234 | 4 | -4 6 2 | 71.19 |
| 1.2785 | 1 | 0 8 3 | 74.10 |
| 1.2722 | 1L | 1 11 1 | 74.53 |
| 1.2674 | 1L | 0 12 0 | 74.86 |
| 1.2481M | 3 | 4 6 0 | 76.22 |
| 1.2481M | | -4 0 4 | 76.22 |
| 1.2441 | 2 | 2 10 1 | 76.51 |
| 1.2336 | 3 | 2 8 2 | 77.28 |
| 1.2309+ | 2 | -4 2 4 | 77.48 |
| 1.2309+ | | 0 12 1 | 77.48 |

Calcium Tin Oxide, CaSnO_3

Synonym

1. Calcium stannate

CAS registry no.

12013-46-6

Sample

The sample was obtained from CERAC, Inc. Milwaukee, WI. The material was heated to 800 °C for one hour. A small amount of SnO_2 was present in the sample.

Color

White

Structure

Orthorhombic, $\text{P2}_1\text{2}_1\text{2}_1$ (19), $Z = 4$. The structure of CaSnO_3 was studied by Smith and Welch [1960].

Lattice constants of this sample

$a = 5.6615(5) \text{ \AA}$

$b = 7.8825(7)$

$c = 5.5162(5)$

$a/b = 0.7182$

$c/b = 0.6998$

Volume

246.17 \AA^3

Density

(calculated) 5.579 g/cm^3

Figure of merit

$F_{30} = 55.5(0.011,51)$

Reference intensity

$I/I_{\text{corundum}} = 6.5(4)$

Additional patterns

1. PDF card 3-755 [H. D. Megaw, Philips Lamps Ltd.]
2. Coughanour et al. [1955]

References

- Coughanour, L. W., Roth, R. S., Marzullo, S., and Sennett, F. E. (1955). J. Res. Nat. Bur. Stand. 54, No. 3, 149.
Smith, A. J. and Welch, A. J. E. (1960). Acta. Crystallogr. 13, 653.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$ | | | |
|---|--------------------------------------|-------|---------------------|
| Internal standard W, $a = 3.16524 \text{ \AA}$ | | | |
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 1$ | hkl | $2\theta(^{\circ})$ |
| 3.943 | 60 | 0 2 0 | 22.53 |
| 3.531 | 2 | 1 1 1 | 25.20 |
| 2.830 | 26 | 2 0 0 | 31.59 |
| 2.789 | 100 | 1 2 1 | 32.07 |
| 2.758 | 23 | 0 0 2 | 32.44 |

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 1$ | hkl | $2\theta(^{\circ})$ |
|-----------------|--------------------------------------|-------|---------------------|
| 2.518 | 1L | 2 0 1 | 35.62 |
| 2.480 | 1 | 1 0 2 | 36.19 |
| 2.398 | 1 | 2 1 1 | 37.47 |
| 2.371 | 3 | 0 3 1 | 37.91 |
| 2.366 | 3 | 1 1 2 | 38.00 |
| 2.298 | 3 | 2 2 0 | 39.17 |
| 2.259 | 3 | 0 2 2 | 39.87 |
| 2.188 | 2 | 1 3 1 | 41.22 |
| 2.122 | 1 | 2 2 1 | 42.56 |
| 2.099 | 1L | 1 2 2 | 43.06 |
| 1.9751 | 32 | 2 0 2 | 45.91 |
| 1.9714 | 29 | 0 4 0 | 46.00 |
| 1.9256 | 1 | 2 3 0 | 47.16 |
| 1.9168 | 1 | 2 1 2 | 47.39 |
| 1.8183 | 1L | 2 3 1 | 50.13 |
| 1.8038 | 1L | 1 3 2 | 50.56 |
| 1.7853 | 7 | 3 0 1 | 51.12 |
| 1.7638 | 19 | 1 4 1 | 51.79 |
| 1.7484 | 4 | 1 0 3 | 52.28 |
| 1.7076 | 1 | 1 1 3 | 53.63 |
| 1.6266 | 15 | 3 2 1 | 56.53 |
| 1.6177 | 12 | 2 4 0 | 56.87 |
| 1.6030 | 15 | 0 4 2 | 57.44 |
| 1.5984 | 23 | 1 2 3 | 57.62 |
| 1.5420M | 1L | 1 4 2 | 59.94 |
| 1.5420M | | 2 0 3 | 59.94 |
| 1.4766 | 1 | 3 3 1 | 62.89 |
| 1.4155 | 2 | 4 0 0 | 65.94 |
| 1.3951 | 2 | 2 4 2 | 67.03 |
| 1.3788 | 10 | 0 0 4 | 67.93 |
| 1.3393M | 1L | 1 0 4 | 70.22 |
| 1.3393M | | 3 3 2 | 70.22 |
| 1.3362 | 1 | 2 5 1 | 70.41 |
| 1.3320 | 2 | 4 2 0 | 70.66 |
| 1.3301M | 2 | 1 5 2 | 70.78 |
| 1.3301M | | 2 3 3 | 70.78 |
| 1.3231 | 4 | 3 4 1 | 71.21 |
| 1.3173 | 2 | 3 0 3 | 71.57 |
| 1.3082 | 2 | 1 4 3 | 72.15 |
| 1.3021 | 1 | 0 2 4 | 72.54 |
| 1.2592 | 2 | 4 0 2 | 75.43 |
| 1.2489 | 7 | 3 2 3 | 76.16 |
| 1.2466M | 9 | 1 6 1 | 76.33 |
| 1.2466M | | 4 3 0 | 76.33 |
| 1.2398 | 3 | 2 0 4 | 76.82 |
| 1.2324 | 1L | 2 5 2 | 77.37 |
| 1.2247 | 1L | 2 1 4 | 77.95 |
| 1.2144 | 1L | 2 4 3 | 78.74 |
| 1.1994 | 2 | 4 2 2 | 79.92 |
| 1.1966 | 2 | 0 5 3 | 80.14 |

Calcium Tin Oxide, CaSnO_3 - (continued)

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 1$ | hkl | $2\theta(^{\circ})$ |
|-----------------|--------------------------------------|-------|---------------------|
| 1.1916 | 1 | 2 6 0 | 80.55 |
| 1.1861 | 1 | 0 6 2 | 81.00 |
| 1.1825 | 3 | 2 2 4 | 81.30 |
| 1.1708 | 1L | 1 5 3 | 82.28 |
| 1.1499 | 2 | 4 4 0 | 84.12 |
| 1.1358 | 1L | 4 3 2 | 85.41 |
| 1.1300 | 2 | 0 4 4 | 85.95 |
| 1.1092 | 1 | 5 0 1 | 87.97 |
| 1.0948 | 2 | 3 4 3 | 89.43 |
| 1.0939 | 2 | 2 6 2 | 89.53 |

Cerium Nitrate Hydrate, $\text{Ce}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$

Synonym

1. Cerous nitrate hexahydrate

CAS registry no.

10294-41-4

Sample

The sample was obtained from the Fisher Scientific Co., Fair Lawn, NJ.

Color

Colorless

Structure

Triclinic, $\bar{P}1(2)$, $Z = 2$. The structure of $\text{Ce}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ was studied by Iveronova et al. [1955].

Lattice constants of this sample

$a = 8.905(2) \text{ \AA}$

$b = 10.683(3)$

$c = 6.6182(14)$

$\alpha = 101.18(2)^\circ$

$\beta = 102.19(2)$

$\gamma = 87.89(2)$

$a/b = 0.8336$

$c/b = 0.6195$

Volume

603.7 \AA^3

Density

(calculated 2.389 g/cm^3)

Figure of merit

$F_{30} = 45.8(0.013, 51)$

Reference intensity

$I/I_{\text{corundum}} = 0.44(3)$

Additional pattern

1. PDF card 14-3 [Hanawalt et al., 1938]

References

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

Iveronova, V. I., Tarasova, V. P., Zolina, Z. K., Markhasin, G. V., and Sukhodereva, I. M. (1955). Zh. Fiz. Khim. 29, 314.

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 5$ | hkl | $2\theta(^\circ)$ |
|-----------------|--------------------------------------|---------|-------------------|
| 5.437 | 42 | -1 -1 1 | 16.29 |
| 5.245 | 42 | 0 2 0 | 16.89 |
| 5.024 | 44 | 0 1 1 | 17.64 |
| 4.701 | 100 | -1 1 1 | 18.86 |
| 4.487M | 39 | 0 -2 1 | 19.77 |
| 4.487M | | 1 2 0 | 19.77 |
| 4.358 | 46 | 2 0 0 | 20.36 |
| 4.017 | 22 | 2 1 0 | 22.11 |
| 4.001 | 27 | -2 0 1 | 22.20 |
| 3.890 | 14 | -2 -1 1 | 22.84 |
| 3.770 | 19 | 1 -2 1 | 23.58 |
| 3.711 | 6 | 0 2 1 | 23.96 |
| 3.576 | 4 | -1 2 1 | 24.88 |
| 3.493 | 2 | 0 3 0 | 25.48 |
| 3.375 | 28 | -2 -2 1 | 26.39 |
| 3.341M | 21 | 0 -3 1 | 26.66 |
| 3.341M | | 2 2 0 | 26.66 |
| 3.247M | 50 | -1 3 0 | 27.45 |
| 3.247M | | -1 -1 2 | 27.45 |
| 3.237M | 33 | 1 3 0 | 27.53 |
| 3.237M | | -1 -3 1 | 27.53 |
| 3.213 | 37 | 0 -1 2 | 27.74 |
| 3.175 | 15 | 0 0 2 | 28.08 |
| 3.048 | 14 | 2 1 1 | 29.28 |
| 3.013M | 25 | 1 -3 1 | 29.63 |
| 3.013M | | -2 2 1 | 29.63 |
| 3.002 | 28 | -1 -2 2 | 29.74 |
| 2.979 | 29 | 0 -2 2 | 29.97 |
| 2.913 | 45 | -1 1 2 | 30.67 |
| 2.892M | 47 | -2 -1 2 | 30.89 |
| 2.892M | | 0 1 2 | 30.89 |
| 2.875 | 11 | -3 0 1 | 31.08 |
| 2.864 | 11 | -2 0 2 | 31.20 |
| 2.839 | 31 | 0 3 1 | 31.49 |
| 2.832M | 28 | -3 -1 1 | 31.57 |
| 2.832M | | 1 -1 2 | 31.57 |
| 2.802M | 11 | 1 0 2 | 31.91 |
| 2.802M | | -3 1 0 | 31.91 |
| 2.794M | 15 | -2 -3 1 | 32.01 |
| 2.794M | | 3 1 0 | 32.01 |
| 2.715+ | 21 | -3 1 1 | 32.96 |
| 2.715+ | | -2 -2 2 | 32.96 |
| 2.663M | 19 | 1 -2 2 | 33.63 |
| 2.663M | | 2 2 1 | 33.63 |
| 2.651 | 35 | -2 1 2 | 33.78 |
| 2.620 | 28 | 0 4 0 | 34.19 |
| 2.611M | 30 | -3 -2 1 | 34.32 |
| 2.611M | | 0 -3 2 | 34.32 |
| 2.550 | 19 | -1 -4 1 | 35.16 |
| 2.542 | 14 | -3 2 0 | 35.28 |

$\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$

Internal standard Si, $a = 5.43088 \text{ \AA}$

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 5$ | hkl | $2\theta(^\circ)$ |
|-----------------|--------------------------------------|--------|-------------------|
| 8.70 | 21 | 1 0 0 | 10.16 |
| 6.71 | 85 | -1 1 0 | 13.19 |
| 6.37 | 60 | 0 0 1 | 13.90 |
| 5.96 | 76 | 0 -1 1 | 14.85 |
| 5.73 | 54 | -1 0 1 | 15.44 |

Cerium Nitrate Hydrate, $\text{Ce}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ - (continued)

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 5$ | hkl | $2\theta(^{\circ})$ |
|-----------------|--------------------------------------|---------|---------------------|
| 2.533 | 18 | 3 2 0 | 35.41 |
| 2.527M | 24 | -1 2 2 | 35.49 |
| 2.527M | | 2 -3 1 | 35.49 |
| 2.490 | 18 | -2 3 1 | 36.04 |
| 2.452 | 20 | 3 0 1 | 36.62 |
| 2.440 | 15 | 1 -4 1 | 36.80 |
| 2.424 | 13 | -2 -3 2 | 37.05 |
| 2.405 | 13 | -3 0 2 | 37.36 |
| 2.393 | 5 | 1 -3 2 | 37.56 |
| 2.359 | 6 | 2 -1 2 | 38.12 |
| 2.352 | 12 | -2 2 2 | 38.24 |
| 2.316M | 23 | -2 -4 1 | 38.85 |
| 2.316M | | -3 -3 1 | 38.85 |
| 2.313M | 26 | -3 -2 2 | 38.91 |
| 2.313M | | 1 2 2 | 38.91 |
| 2.291 | 32 | 3 -2 1 | 39.30 |
| 2.280 | 31 | 2 3 1 | 39.49 |
| 2.265 | 14 | 2 -2 2 | 39.77 |
| 2.249M | 28 | -1 -4 2 | 40.06 |
| 2.249M | | -2 4 0 | 40.06 |
| 2.243M | 24 | -1 4 1 | 40.17 |
| 2.243M | | 0 -4 2 | 40.17 |
| 2.227 | 5 | 3 3 0 | 40.47 |
| 2.204M | 19 | -1 -1 3 | 40.91 |
| 2.204M | | -4 0 1 | 40.91 |
| 2.184 | 13 | -4 -1 1 | 41.31 |
| 2.159+ | 27 | 1 4 1 | 41.80 |
| 2.159+ | | 3 2 1 | 41.80 |
| 2.153M | 27 | 0 3 2 | 41.92 |
| 2.153M | | -1 -2 3 | 41.92 |
| 2.137 | 22 | -3 3 1 | 42.26 |
| 2.129M | 26 | -4 1 1 | 42.43 |
| 2.129M | | 4 1 0 | 42.43 |
| 2.116M | 35 | 0 0 3 | 42.70 |
| 2.116M | | 0 -5 1 | 42.70 |
| 2.107 | 28 | 0 -2 3 | 42.89 |
| 2.088 | 20 | 2 -3 2 | 43.29 |
| 2.081 | 20 | -2 0 3 | 43.44 |
| 2.077M | 21 | -3 2 2 | 43.53 |
| 2.077M | | -4 -2 1 | 43.53 |
| 2.053 | 11 | -2 3 2 | 44.08 |
| 2.039 | 22 | -1 5 0 | 44.39 |
| 2.035M | 17 | 1 5 0 | 44.49 |
| 2.035M | | 2 2 2 | 44.49 |
| 2.024+ | 6 | 1 -5 1 | 44.74 |
| 2.024+ | | 1 3 2 | 44.74 |
| 2.012 | 3 | -4 2 0 | 45.01 |
| 1.999 | 19 | -4 0 2 | 45.33 |
| 1.987M | 8 | -4 2 1 | 45.63 |
| 1.987M | | 0 -3 3 | 45.63 |
| 1.973 | 10 | -2 1 3 | 45.97 |

Chromium Boride, ζ -CrB

CAS registry no.
12006-79-0

Sample

The sample was obtained from Cerac, Menomonee Falls, WI.

Color

Metallic gray

Structure

Orthorhombic, Cmc \bar{m} (63), Z = 4. The structure was determined by Kiessling [1949].

Lattice constants of this sample

$a = 2.9663(4) \text{ \AA}$
 $b = 7.8666(10)$
 $c = 2.9322(5)$

$a/b = 0.3771$
 $c/b = 0.3727$

Volume

68.422 \AA^3

Density

(calculated) 6.097 g/cm^3

Figure of merit

$F_{19} = 62.9(0.013, 24)$

Reference intensity

$I/I_{\text{corundum}} = 1.22(8)$

Polymorphism

Papesch et al., [1973] also observed a tetragonal low temperature form of CrB with 52-56 atom % B.

Additional pattern

1. PDF card 9-361 [Plessey Co. Ltd., Caswell, Towcester, Northants, England].

References

Kiessling, R. (1949). Acta Chem. Scand. 3, 595.
Papesch, G., Nowotny, H., and Benesovsky, F. (1973). Monatsh. Chem. 104, 933.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$ Internal standard W, $a = 3.16524 \text{ \AA}$ | | | |
|---|--------------------------------------|-------|-------------------|
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 6$ | hkl | $2\theta(^\circ)$ |
| 3.936 | 5 | 0 2 0 | 22.57 |
| 2.776 | 38 | 1 1 0 | 32.22 |
| 2.351 | 74 | 0 2 1 | 38.25 |
| 2.016 | 100 | 1 1 1 | 44.92 |
| 1.965M | 79 | 0 4 0 | 46.15 |
| 1.965M | | 1 3 0 | 46.15 |
| 1.6322 | 32 | 1 3 1 | 56.32 |
| 1.4829 | 14 | 2 0 0 | 62.59 |
| 1.4663 | 17 | 0 0 2 | 63.38 |
| 1.3881 | 1L | 2 2 0 | 67.41 |
| 1.3111 | 6 | 0 6 0 | 71.96 |
| 1.2961 | 12 | 1 1 2 | 72.93 |
| 1.2555 | 34 | 1 5 1 | 75.69 |
| 1.2543 | 30 | 2 2 1 | 75.78 |
| 1.1970 | 9 | 0 6 1 | 80.11 |
| 1.1840 | 12 | 2 4 0 | 81.17 |
| 1.1752M | 30 | 0 4 2 | 81.91 |
| 1.1752M | | 1 3 2 | 81.91 |
| 1.0980 | 13 | 2 4 1 | 89.10 |
| 1.0509 | 13 | 1 7 0 | 94.27 |
| 1.0427 | 14 | 2 0 2 | 95.25 |

Chromium Chloride CrCl₃

Synonyms

1. Chromic chloride
2. Chromium trichloride

CAS registry no.

10025-73-7

Sample

The sample was obtained from Fisher Scientific Co., Fair Lawn, N.J.

Color

Deep purple red.

Structure

Monoclinic, A2/m (12), Z = 4, pseudo-hexagonal. The structure was determined by Morosin and Narath [1964]. This form exists at room temperature.

Lattice constants of this sample

a = 6.123(2) Å
b = 10.311(3)
c = 5.956(5)
β = 108.64(5)°

a/b = 0.5938
c/b = 0.5776

Volume

356.3 Å³

Density

(calculated) 2.952 g/cm³

Figures of merit

F₁₉ = 13.2 (0.018,80)
M₁₉ = 16.0

Reference intensity

I/I_{corundum} = 4.5(2)

Polymorphism

There is a hexagonal form found by Wooster [1930] and a low temperature form also found by Morosin and Narath [1964].

Additional pattern

1. PDF card 6-535 [Handy and Gregory, 1952]

References

- Handy, L. L. and Gregory, N. W. (1952). J. Am. Chem. Soc. 74, 891.
Morosin, B. and Narath, A. (1964). J. Chem. Phys. 40, 1958.
Wooster, N. (1930). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 74, 363.

| CuK α_1 λ = 1.540598 Å; temp. 25 \pm 1 °C | | | | |
|--|------------------|--------|----------------|--|
| Internal standard W, a = 3.16524 Å | | | | |
| d(Å) | I ^{rel} | hkl | 2 θ (°) | |
| σ = \pm 3 | | | | |
| 5.80 | 100 | 1 0 0 | 15.27 | |
| 5.154 | 1 | 0 2 0 | 17.19 | |
| 3.849 | 1L | 1 2 0 | 23.09 | |
| 2.936M | 2 | 0 3 1 | 30.42 | |
| 2.936M | | -1 0 2 | 30.42 | |
| 2.901 | 14 | 2 0 0 | 30.80 | |
| 2.816 | 1 | 0 0 2 | 31.75 | |
| 2.577 | 1 | 0 4 0 | 34.78 | |
| 2.475 | 2 | 0 2 2 | 36.27 | |
| 2.460 | 6 | 1 3 1 | 36.49 | |
| 1.934 | 1 | 3 0 0 | 46.94 | |
| 1.911 | 1 | 2 3 1 | 47.54 | |
| 1.754 | 3 | -3 3 1 | 52.09 | |
| 1.720 | 3 | -1 3 3 | 53.21 | |
| 1.6511M | 1 | 3 1 1 | 55.62 | |
| 1.6511M | | 0 3 3 | 55.62 | |
| 1.6478M | 1 | 1 6 0 | 55.74 | |
| 1.5039 | 1L | 3 3 1 | 61.62 | |
| 1.4498M | 6 | -3 5 1 | 64.19 | |
| 1.4498M | | 4 0 0 | 64.19 | |
| 1.4115M | 1 | 0 0 4 | 66.15 | |
| 1.4115M | | -2 2 4 | 66.15 | |
| 1.3954M | 1 | 4 2 0 | 67.01 | |
| 1.3954M | | -4 3 1 | 67.01 | |

Chromium Iron Oxide, $\text{Cr}_{1.3}\text{Fe}_{0.7}\text{O}_3$

Sample

The sample was obtained from the City Chemical Corp., New York, N. Y. It was labelled iron chromite (FeCr_2O_4). The approximate composition was determined by the relation of the cell parameters to those of Fe_2O_3 and Cr_2O_3 . This is a solid solution between hematite (Fe_2O_3) and chromic oxide (Cr_2O_3).

Color

Dark brown

Structure

Hexagonal, $R\bar{3}c$ (167), $Z = 6$. The structure of Cr_2O_3 was determined by Wretblad [1930]. The structure of hematite (Fe_2O_3) was determined by Davey [1923].

Lattice constants of this sample

$a = 4.9965(6) \text{ \AA}$
 $c = 13.621(3)$

$c/a = 2.7261$

Volume

294.49 \AA^3

Density

(calculated) 5.233 g/cm^3

Figure of merit

$F_{20} = 51.0(0.014, 29)$

Reference intensity

$I/I_{\text{corundum}} = 2.11(8)$

References

Davey, W. P. (1923). Phys. Rev. 21, 716.
Wretblad, P. E. (1930). Z. Anorg. Chem. 189, 329.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$ Internal standard Si, $a = 5.43088 \text{ \AA}$ | | | |
|--|--------------------------------------|--------|-------------------|
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 3$ | hkl | $2\theta(^\circ)$ |
| 3.654 | 43 | 0 1 2 | 24.34 |
| 2.676 | 100 | 1 0 4 | 33.46 |
| 2.499 | 73 | 1 1 0 | 35.90 |
| 2.270 | 4 | 0 0 6 | 39.67 |
| 2.189 | 27 | 1 1 3 | 41.21 |
| 2.063 | 4 | 2 0 2 | 43.85 |
| 1.8268 | 33 | 0 2 4 | 49.88 |
| 1.6801 | 66 | 1 1 6 | 54.58 |
| 1.5896 | 5 | 1 2 2 | 57.97 |
| 1.5849 | 6 | 0 1 8 | 58.16 |
| 1.4738 | 23 | 2 1 4 | 63.02 |
| 1.4421 | 25 | 3 0 0 | 64.57 |
| 1.3380 | 1 | 2 0 8 | 70.30 |
| 1.2988 | 12 | 1 0 10 | 72.75 |
| 1.2488 | 6 | 2 2 0 | 76.17 |
| 1.2179 | 3 | 3 0 6 | 78.47 |
| 1.1794 | 2 | 1 2 8 | 81.56 |
| 1.1528 | 4 | 0 2 10 | 83.86 |
| 1.1319 | 7 | 1 3 4 | 85.77 |
| 1.0945 | 7 | 2 2 6 | 89.46 |

Chromium Oxide, CrO₃

Synonyms

1. Chromic acid anhydride
2. Chromium trioxide

CAS registry no.

1333-82-0

Sample

The sample was from J. T. Baker Chemical Co.,
Phillipsburg, NJ.

Color

Dark reddish brown.

Structure

Orthorhombic, Ama2 (40), Z = 4. The structure
of CrO₃ was studied by Bräkken [1931] and
refined by Byström and Wilhelmi [1950].

Lattice constants of this sample

a = 5.7494(15) Å

b = 8.556(2)

c = 4.7961(11)

a/b = 0.6720

c/b = 0.5606

Volume

235.93 Å³

Density

(calculated) 2.815 g/cm³

Figure of merit

F₃₀ = 56.8(0.016,32)

Reference intensity

I/I_{corundum} = 1.41(13)

Additional pattern

1. PDF card 9-47 [Byström and Wilhelmi, 1950]

References

Bräkken, H. (1931). Z. Kristallogr. Kristall-
geometrie Kristallphys. Kristallchem. 78,
484.

Byström, A. and Wilhelmi, K.-A. (1950). Acta
Chem. Scand., 4, 1131.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$ | | | | | |
|---|------------------|-------|---|---|---------------------|
| Internal standard Si, $a = 5.43088 \text{ \AA}$ | | | | | |
| $d(\text{\AA})$ | I^{rel} | hkl | | | $2\theta(^{\circ})$ |
| $\sigma = \pm 3$ | | | | | |
| 4.279 | 19 | 0 | 2 | 0 | 20.74 |
| 4.186 | 90 | 0 | 1 | 1 | 21.21 |
| 3.435 | 100 | 1 | 2 | 0 | 25.92 |
| 3.383 | 64 | 1 | 1 | 1 | 26.32 |
| 2.874 | 44 | 2 | 0 | 0 | 31.09 |
| | | | | | |
| 2.454 | 4 | 0 | 3 | 1 | 36.59 |
| 2.398 | 17 | 0 | 0 | 2 | 37.48 |
| 2.370 | 18 | 2 | 1 | 1 | 37.94 |
| 2.255 | 18 | 1 | 3 | 1 | 39.94 |
| 2.139 | 2 | 0 | 4 | 0 | 42.21 |
| | | | | | |
| 2.091 | 2 | 0 | 2 | 2 | 43.23 |
| 2.006 | 8 | 1 | 4 | 0 | 45.17 |
| 1.966 | 10 | 1 | 2 | 2 | 46.14 |
| 1.866 | 2 | 2 | 3 | 1 | 48.77 |
| 1.842 | 5 | 2 | 0 | 2 | 49.43 |
| | | | | | |
| 1.749 | 10 | 3 | 2 | 0 | 52.26 |
| 1.743 | 11 | 3 | 1 | 1 | 52.44 |
| 1.7168 | 5 | 2 | 4 | 0 | 53.32 |
| 1.6921 | 3 | 2 | 2 | 2 | 54.16 |
| 1.6112 | 3 | 0 | 5 | 1 | 57.12 |
| | | | | | |
| 1.5954 | 2 | 0 | 4 | 2 | 57.74 |
| 1.5706 | 3 | 0 | 1 | 3 | 58.74 |
| 1.5512 | 1 | 1 | 5 | 1 | 59.55 |
| 1.5380 | 2 | 1 | 4 | 2 | 60.11 |
| 1.5159 | 4 | 1 | 1 | 3 | 61.08 |
| | | | | | |
| 1.5097 | 4 | 3 | 3 | 1 | 61.36 |
| 1.4366 | 6 | 4 | 0 | 0 | 64.85 |
| 1.4262 | 3 | 0 | 6 | 0 | 65.38 |
| 1.4124 | 4 | 3 | 2 | 2 | 66.10 |
| 1.4062 | 6 | 2 | 5 | 1 | 66.43 |
| | | | | | |
| 1.3956 | 3 | 2 | 4 | 2 | 67.00 |
| 1.3795 | 5 | 2 | 1 | 3 | 67.89 |
| 1.3555 | 6 | 1 | 3 | 3 | 69.26 |
| 1.2773 | 2 | 2 | 6 | 0 | 74.18 |

Cinchonine, C₁₉H₂₂N₂O

Synonym

1. (9S)-Cinchonan-9-ol

CAS registry no.

118-10-5

Sample

The sample was obtained from the Eastman Kodak Co., Rochester, N. Y. It was recrystallized from ethanol.

Color

Colorless

Structure

Monoclinic, P2₁/*, Z = 2. The unit cell and space group were determined by Paretzkin [1956].

Lattice constants of this sample

a = 11.091(2) Å

b = 7.200(3)

c = 10.774(2)

β = 107.95(2)°

a/b = 1.5404

c/b = 1.4964

Volume

818.48 Å³

Density

(calculated) 1.195 g/cm³

Figure of merit

F₃₀ = 46.6(0.012,52)

Additional pattern

1. PDF card 7-526 [Paretzkin, Polytechnic Institute of Brooklyn].

References

Paretzkin, B. (1956). Acta Crystallogr. 9, 290.

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C Internal standard Si, a = 5.43088 Å | | | | |
|--|----------------------------|--------|-------|--|
| d(Å) | I ^{rel} σ = ±2 | hkl | 2θ(°) | |
| 10.53 | 100 | 1 0 0 | 8.39 | |
| 8.84 | 1L | -1 0 1 | 10.00 | |
| 6.43 | 2 | 1 0 1 | 13.76 | |
| 5.898 | 10 | 0 1 1 | 15.01 | |
| 5.583 | 1 | -1 1 1 | 15.86 | |
| 5.417 | 4 | -2 0 1 | 16.35 | |
| 5.301 | 20 | -1 0 2 | 16.71 | |
| 5.282 | 24 | 2 0 0 | 16.77 | |
| 5.119 | 19 | 0 0 2 | 17.31 | |
| 4.795 | 4 | 1 1 1 | 18.49 | |
| 4.423 | 3 | -2 0 2 | 20.06 | |
| 4.327 | 5 | -2 1 1 | 20.51 | |
| 4.251 | 7 | 2 1 0 | 20.88 | |
| 4.197 | 21 | 2 0 1 | 21.15 | |
| 4.135 | 10 | 1 0 2 | 21.47 | |
| 3.770 | 2 | -2 1 2 | 23.58 | |
| 3.623 | 10 | 2 1 1 | 24.55 | |
| 3.586M | 3 | -1 0 3 | 24.81 | |
| 3.586M | | 1 1 2 | 24.81 | |
| 3.437 | 1L | -3 0 2 | 25.90 | |
| 3.409 | 1L | 1 2 0 | 26.12 | |
| 3.288 | 1L | -3 1 1 | 27.10 | |
| 3.213M | 1 | 2 0 2 | 27.74 | |
| 3.213M | | -1 1 3 | 27.74 | |
| 3.161 | 1 | 3 1 0 | 28.21 | |
| 3.102 | 1 | -3 1 2 | 28.76 | |
| 3.089 | 1 | 0 1 3 | 28.88 | |
| 3.049 | 1L | 3 0 1 | 29.27 | |
| 2.936 | 2 | 2 1 2 | 30.42 | |
| 2.809 | 2 | 3 1 1 | 31.83 | |
| 2.770 | 1L | -4 0 1 | 32.29 | |
| 2.761 | 1L | 1 1 3 | 32.40 | |
| 2.726 | 1L | -3 1 3 | 32.83 | |
| 2.708 | 1L | -4 0 2 | 33.05 | |
| 2.687 | 1 | -1 0 4 | 33.32 | |
| 2.638 | 1L | 4 0 0 | 33.96 | |
| 2.556 | 1 | 3 0 2 | 35.08 | |
| 2.541 | 1 | -1 2 3 | 35.29 | |
| 2.534M | 1 | -4 1 2 | 35.39 | |
| 2.534M | | 2 0 3 | 35.39 | |
| 2.480 | 1L | 0 2 3 | 36.19 | |
| 2.464M | 1L | -2 2 3 | 36.43 | |
| 2.464M | | -3 0 4 | 36.43 | |
| 2.408 | 1 | 3 1 2 | 37.31 | |
| 2.388 | 1L | 2 1 3 | 37.63 | |

Cinchonine, C₁₉H₂₂N₂O - (continued)

| d(Å) | I ^{rel} σ = ±2 | hkl | 2θ(°) |
|---------|----------------------------|--------|-------|
| 2.328 | 1L | 3 2 1 | 38.64 |
| 2.279 | 1L | -3 2 3 | 39.51 |
| 2.263 | 1L | 4 1 1 | 39.81 |
| 2.218 | 1L | 1 1 4 | 40.65 |
| 2.208 | 1L | -4 0 4 | 40.83 |
| 2.165 | 1L | -4 2 2 | 41.69 |
| 2.140 | 1L | -1 0 5 | 42.19 |
| 2.111+ | 1 | 5 0 0 | 42.80 |
| 2.111+ | | -5 0 3 | 42.80 |
| 2.082 | 1L | 2 3 1 | 43.43 |
| 2.069M | 1L | -3 0 5 | 43.72 |
| 2.069M | | 2 0 4 | 43.72 |
| 2.051+ | 1L | -1 1 5 | 44.12 |
| 2.051+ | | 0 0 5 | 44.12 |
| 2.024M | 1L | 5 1 0 | 44.74 |
| 2.024M | | -5 1 3 | 44.74 |
| 2.012M | 1L | 4 1 2 | 45.02 |
| 2.012M | | -3 3 1 | 45.02 |
| 1.9898 | 1L | -3 1 5 | 45.55 |
| 1.9570M | 1L | -2 3 3 | 46.36 |
| 1.9570M | | 1 2 4 | 46.36 |
| 1.9514M | 1L | 5 0 1 | 46.50 |
| 1.9514M | | -5 0 4 | 46.50 |
| 1.8846M | 1L | 5 1 1 | 48.25 |
| 1.8846M | | -4 2 4 | 48.25 |
| 1.8795M | 1L | -5 2 1 | 48.39 |
| 1.8795M | | -5 2 2 | 48.39 |
| 1.8389 | 1L | -1 2 5 | 49.53 |
| 1.8115 | 1L | 4 2 2 | 50.33 |
| 1.8065 | 1L | -6 0 3 | 50.48 |
| 1.7932 | 1L | 2 2 4 | 50.88 |

Clopenthixol Hydrate, $C_{22}H_{25}ClN_2OS \cdot 2H_2O$

Synonym

1. 4-[3-(2-Chlorothioxanthen-9-ylidene)propyl]
-1-piperazineethanol dihydrate

Sample

The sample was supplied by J. Rodgers, University of Adelaide, Adelaide, South Australia. Chemical analysis gave weight percents indicating that the dihydrate is the most probable formula.

Color

Colorless

Structure

Triclinic, $P\bar{3}$, $Z = 2$. The unit cell was measured on a single crystal diffractometer by V. Himes at NBS (priv. comm.). The value of Z was assumed from the measured density.

Lattice constants of this sample

$a = 7.773(3) \text{ \AA}$
 $b = 21.939(11)$
 $c = 6.518(4)$
 $\alpha = 91.60(5)^\circ$
 $\beta = 93.06(4)$
 $\gamma = 90.06(4)$

$a/b = 0.3543$

$c/b = 0.2971$

Volume

$1110. \text{ \AA}^3$

Density

(calculated) 1.308 g/cm^3

(measured) 1.34 g/cm^3

Figure of merit

$F_{30} = 23.0(0.016, 80)$

Reference intensity

$I/I_{\text{corundum}} = 1.01(5)$

Polymorphism

The form described here is the inactive isomer having no neuroleptic activity. An active isomer also exists.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$ Internal standard Ag, $a = 4.08651 \text{ \AA}$ | | | |
|--|--------------------------------------|---------|-------------------|
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 6$ | hkl | $2\theta(^\circ)$ |
| 22.02 | 100 | 0 1 0 | 4.01 |
| 11.00 | 15 | 0 2 0 | 8.03 |
| 7.32+ | 38 | -1 1 0 | 12.08 |
| 7.32+ | | 1 1 0 | 12.08 |
| 6.29 | 39 | 0 -1 1 | 14.07 |
| 5.65 | 11 | 0 -2 1 | 15.66 |
| 5.48 | 4 | 0 4 0 | 16.15 |
| 5.34 | 16 | -1 3 0 | 16.59 |
| 5.122 | 7 | -1 0 1 | 17.30 |
| 5.012 | 13 | -1 -1 1 | 17.68 |
| 4.792 | 43 | 0 3 1 | 18.50 |
| 4.721 | 33 | 1 1 1 | 18.78 |
| 4.609 | 55 | -1 2 1 | 19.24 |
| 4.405 | 3 | 1 2 1 | 20.14 |
| 4.243 | 12 | -1 -3 1 | 20.92 |
| 4.135 | 4 | 0 4 1 | 21.47 |
| 3.882 | 20 | 2 0 0 | 22.89 |
| 3.824+ | 18 | -2 1 0 | 23.24 |
| 3.824+ | | -1 5 0 | 23.24 |
| 3.703 | 12 | -1 4 1 | 24.01 |
| 3.658+ | 45 | -2 2 0 | 24.31 |
| 3.658+ | | 2 2 0 | 24.31 |
| 3.597 | 7 | 1 4 1 | 24.73 |
| 3.431 | 32 | -2 3 0 | 25.95 |
| 3.371M | 44 | -2 1 1 | 26.42 |
| 3.371M | | -1 -5 1 | 26.42 |
| 3.294 | 17 | 1 -5 1 | 27.05 |
| 3.269 | 21 | -2 -2 1 | 27.26 |
| 3.248M | 19 | 0 0 2 | 27.44 |
| 3.248M | | -2 2 1 | 27.44 |
| 3.221M | 15 | 0 -6 1 | 27.67 |
| 3.221M | | 1 5 1 | 27.67 |
| 3.167M | 11 | -2 4 0 | 28.15 |
| 3.167M | | 2 4 0 | 28.15 |
| 3.136M | 10 | 2 -2 1 | 28.44 |
| 3.136M | | 0 7 0 | 28.44 |
| 3.094 | 4 | 0 2 2 | 28.83 |
| 2.993 | 8 | 2 -3 1 | 29.83 |
| 2.960 | 6 | 2 3 1 | 30.17 |
| 2.941M | 5 | 1 0 2 | 30.37 |
| 2.941M | | 0 3 2 | 30.37 |
| 2.795M | 4 | -1 3 2 | 32.00 |
| 2.795M | | 0 7 1 | 32.00 |
| 2.780 | 3 | 2 4 1 | 32.17 |
| 2.740 | 1 | 0 8 0 | 32.66 |

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 6$ | hkl | $2\theta(^{\circ})$ |
|-----------------|--------------------------------------|--------|---------------------|
| 2.678 | 6 | -2 5 1 | 33.43 |
| 2.643 | 3 | -1 4 2 | 33.89 |
| 2.516 | 1 | 3 2 0 | 35.66 |
| 2.449M | 1 | 2 -6 1 | 36.66 |
| 2.449M | | -3 0 1 | 36.66 |
| 2.440+ | 1 | -3 3 0 | 36.81 |
| 2.440+ | | -2 7 0 | 36.81 |
| 2.317M | 5 | -1 6 2 | 38.84 |
| 2.317M | | -3 3 1 | 38.84 |
| 2.299M | 5 | -2 4 2 | 39.15 |
| 2.299M | | 3 2 1 | 39.15 |
| 2.237 | 4 | 2 8 0 | 40.29 |

Copper Hydroxide Phosphate (Libethenite), $\text{Cu}_2(\text{OH})\text{PO}_4$

Synonym

1. Copper phosphate hydrate

CAS registry no.

1318-84-9

Sample

The sample was prepared at NBS by D. Misra by reaction of hydroxyapatite with $\text{Cu}(\text{NO}_3)_2$ solution. The material was dried at 55 °C.

Color

Light yellow green

Structure

Orthorhombic, Pnnm (58), $Z = 4$. The lattice constants of libethenite were determined by Strunz [1936]. The structure was determined by Heritsch [1940].

Lattice constants of this sample

$a = 8.0678(10) \text{ \AA}$

$b = 8.4100(15)$

$c = 5.8896(7)$

$a/b = 0.9593$

$c/b = 0.7003$

Volume

399.61 \AA^3

Density

(calculated) 3.974 g/cm^3

Figure of merit

$F_{30} = 53.6(0.012, 45)$

Reference intensity

$I/I_{\text{corundum}} = 1.13(4)$

Additional patterns

1. PDF card 8-107 [Strunz, 1936]

2. PPF card 1-274 [Hanawalt et al., 1938]

References

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

Heritsch, H. (1940). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 102, 1.

Strunz, H. (1936). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 94, 63.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$ Internal standard Ag, $a = 4.08651 \text{ \AA}$ | | | |
|--|--------------------------------------|-------|-------------------|
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 3$ | hkl | $2\theta(^\circ)$ |
| 5.813 | 93 | 1 1 0 | 15.23 |
| 4.818 | 100 | 0 1 1 | 18.40 |
| 4.751 | 68 | 1 0 1 | 18.66 |
| 4.137 | 6 | 1 1 1 | 21.46 |
| 3.729 | 42 | 1 2 0 | 23.84 |
| 3.638 | 15 | 2 1 0 | 24.45 |
| 2.946 | 18 | 0 0 2 | 30.32 |
| 2.912 | 72 | 2 2 0 | 30.68 |
| 2.647 | 43 | 1 3 0 | 33.84 |
| 2.627 | 61 | 1 1 2 | 34.10 |
| 2.610 | 19 | 2 2 1 | 34.33 |
| 2.561 | 25 | 3 1 0 | 35.01 |
| 2.532 | 10 | 0 3 1 | 35.43 |
| 2.446 | 11 | 3 0 1 | 36.71 |
| 2.414M | 26 | 1 3 1 | 37.21 |
| 2.414M | | 0 2 2 | 37.21 |
| 2.377 | 21 | 2 0 2 | 37.81 |
| 2.348 | 10 | 3 1 1 | 38.30 |
| 2.312 | 21 | 1 2 2 | 38.93 |
| 2.288 | 4 | 2 1 2 | 39.34 |
| 2.265 | 3 | 3 2 0 | 39.77 |
| 2.071 | 6 | 2 2 2 | 43.67 |
| 2.017 | 1 | 4 0 0 | 44.91 |
| 1.9682 | 3 | 1 3 2 | 46.08 |
| 1.9411 | 3 | 3 3 0 | 46.76 |
| 1.9326 | 6 | 3 1 2 | 46.98 |
| 1.9237 | 6 | 1 4 1 | 47.21 |
| 1.9077 | 5 | 1 0 3 | 47.63 |
| 1.8607M | 5 | 4 1 1 | 48.91 |
| 1.8607M | | 1 1 3 | 48.91 |
| 1.8196 | 2 | 4 2 0 | 50.09 |
| 1.8139 | 2 | 2 3 2 | 50.26 |
| 1.7955 | 2 | 3 2 2 | 50.81 |
| 1.7370M | 2 | 4 2 1 | 52.65 |
| 1.7370M | | 1 2 3 | 52.65 |
| 1.7111 | 11 | 0 4 2 | 53.51 |
| 1.6643 | 7 | 4 0 2 | 55.14 |
| 1.6462 | 3 | 1 5 0 | 55.80 |
| 1.6330 | 2 | 4 1 2 | 56.29 |
| 1.6277 | 3 | 2 2 3 | 56.49 |
| 1.6201 | 10 | 3 3 2 | 56.78 |
| 1.5951 | 4 | 3 4 1 | 57.75 |
| 1.5849+ | 9 | 3 0 3 | 58.16 |
| 1.5849+ | | 5 1 0 | 58.16 |
| 1.5767M | 7 | 4 3 1 | 58.49 |

Copper Hydroxide Phosphate (Libethenite), $\text{Cu}_2(\text{OH})\text{PO}_4$ - (continued)

| $d(\text{\AA})$ | I^{rel} | hkl | $2\theta(^{\circ})$ |
|------------------|------------------|-------|---------------------|
| $\sigma = \pm 3$ | | | |
| 1.5767M | | 1 3 3 | 58.49 |
| 1.5590 | 4 | 3 1 3 | 59.22 |
| 1.5472 | 9 | 4 2 2 | 59.72 |
| 1.5302 | 3 | 5 1 1 | 60.45 |
| 1.5063 | 3 | 5 2 0 | 61.51 |
| 1.4724 | 7 | 0 0 4 | 63.09 |
| 1.4554 | 6 | 4 4 0 | 63.91 |
| 1.4276 | 3 | 1 1 4 | 65.31 |

β -L-Glutamic Acid, $C_5H_9NO_4$

Synonyms

1. β -L-glutaminic acid
2. β -L-2-aminopentanedioic acid

CAS registry no.

56-86-0

Sample

The sample was obtained from Sigma Chemical Co., St. Louis, MO.

Color

Colorless

Structure

Orthorhombic, $P2_12_12_1$ (19), $Z = 8$. The structure was determined by Hirokawa [1955].

Lattice constants of this sample

$a = 6.9651(15) \text{ \AA}$

$b = 17.308(3)$

$c = 5.1690(14)$

$a/b = 0.4024$

$c/b = 0.2986$

Volume

623.12 \AA^3

Density

(calculated) 1.568 g/cm^3

Figure of merit

$F_{30} = 48.3(0.016, 39)$

Reference intensity

$I/I_{\text{corundum}} = 0.65(3)$

Polymorphism

There is also an orthorhombic α -form found by Bernal [1931].

References

Bernal, J. D. (1931). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 78, 363.

Hirokawa, S. (1955). Acta Crystallogr. 8, 637.

$\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$
Internal standard Si, $a = 5.43088 \text{ \AA}$

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 3$ | hkl | $2\theta(^{\circ})$ |
|-----------------|--------------------------------------|-------|---------------------|
| 8.65 | 34 | 0 2 0 | 10.22 |
| 6.46 | 10 | 1 1 0 | 13.69 |
| 4.960 | 9 | 0 1 1 | 17.87 |
| 4.445M | 28 | 1 3 0 | 19.96 |
| 4.445M | | 0 2 1 | 19.96 |
| 4.323 | 40 | 0 4 0 | 20.53 |
| 4.155 | 100 | 1 0 1 | 21.37 |
| 4.042 | 75 | 1 1 1 | 21.97 |
| 3.854 | 13 | 0 3 1 | 23.06 |
| 3.746 | 24 | 1 2 1 | 23.73 |
| 3.678 | 10 | 1 4 0 | 24.18 |
| 3.482 | 64 | 2 0 0 | 25.56 |
| 3.415 | 43 | 2 1 0 | 26.07 |
| 3.372 | 6 | 1 3 1 | 26.41 |
| 3.320 | 3 | 0 4 1 | 26.83 |
| 3.232 | 18 | 2 2 0 | 27.58 |
| 3.101 | 10 | 1 5 0 | 28.77 |
| 2.983 | 26 | 2 3 0 | 29.93 |
| 2.887M | 70 | 2 0 1 | 30.95 |
| 2.887M | | 0 6 0 | 30.95 |
| 2.849 | 12 | 2 1 1 | 31.37 |
| 2.741 | 6 | 2 2 1 | 32.64 |
| 2.712 | 12 | 2 4 0 | 33.00 |
| 2.664 | 31 | 1 6 0 | 33.62 |
| 2.583M | 12 | 0 0 2 | 34.70 |
| 2.583M | | 2 3 1 | 34.70 |
| 2.520 | 29 | 0 6 1 | 35.60 |
| 2.475 | 8 | 0 2 2 | 36.27 |
| 2.455 | 4 | 2 5 0 | 36.57 |
| 2.402 | 3 | 2 4 1 | 37.41 |
| 2.398 | 3 | 1 1 2 | 37.47 |
| 2.367 | 12 | 1 6 1 | 37.99 |
| 2.358 | 5 | 0 3 2 | 38.13 |
| 2.330 | 8 | 1 7 0 | 38.61 |
| 2.303 | 2 | 3 1 0 | 39.09 |
| 2.231 | 14 | 0 7 1 | 40.39 |
| 2.154 | 5 | 3 3 0 | 41.91 |
| 2.125 | 6 | 1 7 1 | 42.50 |
| 2.102 | 8 | 3 1 1 | 42.99 |
| 2.057 | 6 | 3 2 1 | 43.98 |

β -L-Glutamic Acid, $C_5H_9NO_4$ - (continued)

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 3$ | hkl | $2\theta(^{\circ})$ |
|-----------------|--------------------------------------|--------|---------------------|
| 2.040 | 8 | 2 6 1 | 44.38 |
| 2.017M | 8 | 2 2 2 | 44.91 |
| 2.017M | | 2 7 0 | 44.91 |
| 1.995 | 3 | 0 8 1 | 45.43 |
| 1.988 | 4 | 3 3 1 | 45.59 |
| 1.953 | 2 | 2 3 2 | 46.47 |
| 1.924 | 3 | 0 6 2 | 47.19 |
| 1.919 | 3 | 1 8 1 | 47.32 |
| 1.902 | 4 | 3 4 1 | 47.79 |
| 1.878 | 4 | 2 7 1 | 48.44 |
| 1.855M | 5 | 1 6 2 | 49.07 |
| 1.855M | | 1 9 0 | 49.07 |
| 1.838 | 1 | 2 8 0 | 49.55 |
| 1.806 | 1 | 3 5 1 | 50.50 |
| 1.803 | 1 | 0 9 1 | 50.59 |
| 1.744 | 3 | 1 9 1 | 52.42 |
| 1.733 | 3 | 4 1 0 | 52.77 |
| 1.729 | 5 | 1 7 2 | 52.90 |
| 1.718 | 4 | 3 1 2 | 53.28 |
| 1.706M | 3 | 3 6 1 | 53.68 |
| 1.706M | | 4 2 0 | 53.68 |
| 1.6921 | 2 | 3 7 0 | 54.16 |
| 1.6838M | 3 | 2 6 2 | 54.45 |
| 1.6838M | | 2 9 0 | 54.45 |
| 1.6640 | 3 | 1 1 3 | 55.15 |
| 1.6588 | 3 | 0 8 2 | 55.34 |
| 1.6505M | 3 | 0 3 3 | 55.64 |
| 1.6505M | | 4 0 1 | 55.64 |
| 1.6421+ | 4 | 4 1 1 | 55.95 |
| 1.6421+ | | 1 2 3 | 55.95 |
| 1.5982 | 3 | 1 10 1 | 57.63 |
| 1.5864 | 2 | 4 3 1 | 58.10 |
| 1.5425M | 2 | 0 9 2 | 59.92 |
| 1.5425M | | 0 5 3 | 59.92 |
| 1.5211 | 2 | 2 2 3 | 60.85 |
| 1.5055M | 1 | 1 5 3 | 61.55 |
| 1.5055M | | 0 11 1 | 61.55 |

Glycine, α -C₂H₅NO₂

Synonym

1. α -Aminoacetic acid

CAS registry no.

56-40-6

Sample

The sample from Fisher Scientific Co., Fair Lawn, NJ. was recrystallized from a mixture of water and methanol to which a small amount of ether was added.

Color

Colorless

Structure

Monoclinic, P2₁/n (14), Z = 4. The structure was determined by Albrecht and Corey [1939] and refined by Marsh [1957].

Lattice constants of this sample

a = 5.4621(12) Å

b = 11.966(3)

c = 5.1077(11)

β = 111.72(2)°

a/b = 0.4565

c/b = 0.4269

Volume

310.14 Å³

Density

(calculated) - .608 g/cm³

Figure of merit

F₃₀ = 40.5 (0.014, 51)

Reference intensity

I/I_{corundum} = 4.6(3)

Polymorphism

α -glycine, the most stable form, is obtained from water at room temperature and below, while β - and γ -glycine are obtained (together with α -glycine) from mixtures of water with acetic acid at higher temperatures [Hubig, 1958].

Additional pattern

1. PDF card 7-718 [Hanawalt et al., 1938]

References

Albrecht, G. and Corey, R. B. (1939). J. Am. Chem. Soc. 61, 1087.
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Hubig, W. Z. (1958). Z. Naturforsch. B13, 633.
Marsh, R. E. (1957). Acta Crystallogr. 10, 814.

| CuK α_1 λ = 1.540598 Å; temp. 25±1 °C | | | |
|--|--------------------------------------|--------|----------------|
| Internal standard W, a = 3.16524 Å | | | |
| d(Å) | I ^{rel} $\sigma = \pm 2$ | hkl | 2 θ (°) |
| 5.98 | 9 | 0 2 0 | 14.80 |
| 4.670 | 9 | 1 1 0 | 18.99 |
| 4.410 | 4 | 0 1 1 | 20.12 |
| 3.874 | 1L | 1 2 0 | 22.94 |
| 3.719 | 15 | 0 2 1 | 23.91 |
| 3.523 | 1L | -1 2 1 | 25.26 |
| 3.134 | 6 | 1 3 0 | 28.46 |
| 3.053 | 10 | 0 3 1 | 29.23 |
| 2.990 | 100 | 0 4 0 | 29.86 |
| 2.874 | 1 | 1 1 1 | 31.09 |
| 2.654 | 1L | 1 2 1 | 33.75 |
| 2.532 | 7 | 0 4 1 | 35.42 |
| 2.481 | 2 | 2 1 0 | 36.18 |
| 2.453 | 4 | -2 2 1 | 36.60 |
| 2.374 | 1L | 0 0 2 | 37.87 |
| 2.336 | 1 | 2 2 0 | 38.50 |
| 2.327 | 1 | 0 1 2 | 38.67 |
| 2.229 | 1L | -2 3 1 | 40.43 |
| 2.205 | 1 | 0 2 2 | 40.90 |
| 2.166 | 1 | 1 5 0 | 41.67 |
| 2.143M | 1 | -1 3 2 | 42.14 |
| 2.143M | | 2 3 0 | 42.14 |
| 2.105 | 1 | 1 4 1 | 42.94 |
| 2.051 | 1L | -2 2 2 | 44.13 |
| 2.039 | 1 | 0 3 2 | 44.40 |
| 2.000 | 1 | -2 4 1 | 45.30 |
| 1.994 | 1 | 0 6 0 | 45.46 |
| 1.935M | 1 | -1 4 2 | 46.91 |
| 1.935M | | 2 4 0 | 46.91 |
| 1.915 | 1 | -2 3 2 | 47.44 |
| 1.874 | 1L | 1 1 2 | 48.54 |
| 1.859M | 1L | 2 2 1 | 48.97 |
| 1.859M | | 0 4 2 | 48.97 |
| 1.839 | 1L | 0 6 1 | 49.54 |
| 1.808 | 1L | 1 2 2 | 50.43 |
| 1.7998 | 1L | -3 1 1 | 50.68 |
| 1.7886 | 1L | -2 5 1 | 51.02 |
| 1.7566 | 1L | 2 3 1 | 52.02 |
| 1.7422M | 1L | -1 5 2 | 52.48 |
| 1.7422M | | -3 2 1 | 52.48 |
| 1.7129 | 1L | 1 3 2 | 53.45 |
| 1.6988 | 1L | -1 0 3 | 53.93 |
| 1.6821 | 1L | -1 1 3 | 54.51 |
| 1.6557 | 1L | -3 3 1 | 55.45 |

Guanidinium Chloride, $\text{CH}_5\text{N}_3\cdot\text{HCl}$

Synonym

1. Guanidine Hydrochloride

CAS registry no.

50-01-1

Sample

The sample was obtained from Mallinckrodt Chemical Works, St. Louis, MO.

Color

Colorless

Structure

Orthorhombic, $\text{Pbca}(61)$, $Z = 8$. The structure was determined by Haas et al. [1965].

Lattice constants of this sample

$a = 9.192(2) \text{ \AA}$

$b = 13.037(4)$

$c = 7.774(2)$

$a/b = 0.7051$

$c/b = 0.5963$

Volume

963.6 \AA^3

Density

(calculated) 1.362 g/cm^3

Figure of merit

$F_{30} = 36.0(0.015, 55)$

Reference intensity

$I/I_{\text{corundum}} = 0.77(2)$

Additional pattern

1. PDF card 3-387 [Theilacker, 1931].

References

Haas, D. J., Harris, D. R., and Mills, H. H. (1965). *Acta Crystallogr.* **19**, 309.

Theilacker, W. (1931). *Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem.* **76**, 203.

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}; \text{ temp. } 25 \pm 1 \text{ } ^\circ\text{C}$ Internal standard W, $a = 3.16524 \text{ \AA}$ | | | | |
|--|--------------------------------------|-------|---------------------|--|
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 1$ | hkl | $2\theta(^{\circ})$ | |
| 4.996 | 3 | 0 2 1 | 17.74 | |
| 4.591 | 13 | 2 0 0 | 19.32 | |
| 4.386 | 88 | 1 2 1 | 20.23 | |
| 4.329 | 16 | 2 1 0 | 20.50 | |
| 3.884 | 9 | 0 0 2 | 22.88 | |
| 3.787 | 46 | 2 1 1 | 23.47 | |
| 3.583 | 50 | 1 0 2 | 24.83 | |
| 3.448 | 96 | 1 1 2 | 25.82 | |
| 3.381 | 54 | 2 2 1 | 26.34 | |
| 3.258 | 29 | 0 4 0 | 27.35 | |
| 2.968 | 100 | 2 0 2 | 30.08 | |
| 2.927 | 12 | 2 3 1 | 30.52 | |
| 2.894 | 5 | 2 1 2 | 30.87 | |
| 2.783 | 31 | 3 1 1 | 32.14 | |
| 2.763 | 41 | 1 3 2 | 32.38 | |
| 2.659 | 75 | 2 4 0 | 33.68 | |
| 2.497 | 35 | 0 4 2 | 35.93 | |
| 2.449M | 10 | 2 3 2 | 36.66 | |
| 2.449M | | 1 1 3 | 36.66 | |
| 2.407M | 11 | 0 2 3 | 37.33 | |
| 2.407M | | 3 0 2 | 37.33 | |
| 2.384 | 6 | 3 3 1 | 37.70 | |
| 2.368 | 2 | 3 1 2 | 37.97 | |
| 2.297 | 13 | 4 0 0 | 39.18 | |
| 2.264 | 5 | 4 1 0 | 39.78 | |
| 2.223 | 2 | 2 1 3 | 40.54 | |
| 2.195 | 9 | 2 4 2 | 41.08 | |
| 2.173M | 4 | 4 1 1 | 41.52 | |
| 2.173M | | 0 6 0 | 41.52 | |
| 2.164 | 4 | 1 3 3 | 41.70 | |
| 2.134 | 3 | 2 2 3 | 42.31 | |
| 2.106M | 11 | 1 5 2 | 42.91 | |
| 2.106M | | 3 3 2 | 42.91 | |
| 2.088 | 9 | 4 2 1 | 43.29 | |
| 2.040 | 4 | 1 6 1 | 44.36 | |
| 2.032 | 1 | 4 3 0 | 44.56 | |
| 1.978 | 3 | 4 0 2 | 45.85 | |
| 1.966M | 5 | 4 3 1 | 46.14 | |
| 1.966M | | 2 6 0 | 46.14 | |
| 1.959 | 7 | 2 5 2 | 46.32 | |
| 1.957M | 5 | 3 1 3 | 46.37 | |
| 1.957M | | 4 1 2 | 46.37 | |
| 1.902 | 6 | 1 0 4 | 47.79 | |
| 1.894M | 6 | 3 2 3 | 47.99 | |
| 1.894M | | 4 2 2 | 47.99 | |

Guanidinium Chloride, $\text{CH}_5\text{N}_3\cdot\text{HCl}$ - (continued)

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 1$ | hkl | | | $2\theta(^{\circ})$ |
|-----------------|--------------------------------------|-----|---|---|---------------------|
| 1.881 | 8 | 1 | 1 | 4 | 48.35 |
| 1.8011M | 5 | 3 | 3 | 3 | 50.64 |
| 1.8011M | | 4 | 3 | 2 | 50.64 |
| 1.7683 | 2 | 3 | 5 | 2 | 51.65 |
| 1.7422 | 7 | 1 | 3 | 4 | 52.48 |
| 1.7279 | 5 | 3 | 6 | 1 | 52.95 |
| 1.7046 | 5 | 4 | 1 | 3 | 53.73 |
| 1.6909M | 6 | 3 | 4 | 3 | 54.20 |
| 1.6909M | | 4 | 4 | 2 | 54.20 |

Hexamethylenetetramine, $C_6H_{12}N_4$

Synonym

1. 1,3,5,7-tetraazatricyclo [3.3.1.1^{3,7}]-decane
2. Methenamine

CAS registry no.

100-97-0

Sample

The sample was obtained from Fisher Scientific Co., Fair Lawn, NJ. It was recrystallized from ethanol. There was one line at $d = 3.152$ with an intensity of 1 that was not accounted for.

Color

Colorless

Structure

Cubic, $I\bar{4}3m$ (217), $Z = 2$. The structure was determined quantitatively by Becka and Cruickshank [1963].

Lattice constant of this sample

$a = 7.0287(3) \text{ \AA}$

Volume

347.24 \AA^3

Density

(calculated) 1.341 g/cm^3

Figure of merit

$F_{22} = 74.3(0.010, 29)$

Reference intensity

$I/I_{\text{corundum}} = 3.84(10)$

Additional pattern

1. PDF card 3-135 [Dow Chemical Co., Midland, MI]

Reference

Becka, L. N. and Cruickshank, D. W. J. (1963). Proc. Roy. Soc. Ser. A 273, 435.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$ Internal standard W, $a = 3.16524 \text{ \AA}$ | | | | | |
|---|------------------|-------|---|---|-------------------|
| $d(\text{\AA})$ | I^{rel} | hkl | | | $2\theta(^\circ)$ |
| $\sigma = \pm 1$ | | | | | |
| 4.968 | 100 | 1 | 1 | 0 | 17.84 |
| 3.517 | 4 | 2 | 0 | 0 | 25.30 |
| 2.870 | 14 | 2 | 1 | 1 | 31.14 |
| 2.485 | 2 | 2 | 2 | 0 | 36.12 |
| 2.224 | 1L | 3 | 1 | 0 | 40.53 |
| 2.0291 | 6 | 2 | 2 | 2 | 44.62 |
| 1.8784 | 4 | 3 | 2 | 1 | 48.42 |
| 1.6560 | 1L | 4 | 1 | 1 | 55.44 |
| 1.5713 | 1L | 4 | 2 | 0 | 58.71 |
| 1.4984 | 1 | 3 | 3 | 2 | 61.87 |
| 1.4346 | 1L | 4 | 2 | 2 | 64.95 |
| 1.3786 | 1 | 5 | 1 | 0 | 67.94 |
| 1.2832 | 1L | 5 | 2 | 1 | 73.78 |
| 1.2424 | 1 | 4 | 4 | 0 | 76.63 |
| 1.2057 | 1L | 5 | 3 | 0 | 79.42 |
| 1.1715 | 1L | 6 | 0 | 0 | 82.22 |
| 1.1404 | 1L | 6 | 1 | 1 | 84.98 |
| 1.0845 | 1L | 5 | 4 | 1 | 90.52 |
| 1.0595 | 1L | 6 | 2 | 2 | 93.28 |
| 1.0362 | 1L | 6 | 3 | 1 | 96.04 |
| .9565 | 1L | 7 | 2 | 1 | 107.29 |
| .8927 | 1L | 7 | 3 | 2 | 119.29 |

Hydrazinium Sulfate, (NH₃)₂SO₄

Synonyms

1. Hydrazine sulfate
2. Hydrazonium sulfate

CAS registry no.

10034-93-2

Sample

Hydrazinium sulfate was obtained from Fisher Scientific Co., Fair Lawn, NJ. It was recrystallized from water. The x-ray pattern was run in a humid atmosphere.

Color

Colorless

Structure

Orthorhombic, P2₁2₁2₁ (19), Z = 4. The structure was determined by Nitta et al. [1951] and refined by Jönsson and Hamilton [1970].

Lattice constants of this sample

a = 8.2579(14) Å

b = 9.178(2)

c = 5.5386(11)

a/b = 0.8997

c/b = 0.6035

Volume

419.78 Å³

Density

(calculated) 2.059 g/cm³

Figure of merit

F₃₀ = 57.4 (0.013, 41)

Reference intensity

I/I_{corundum} = 1.47(8)

Additional pattern

1. PDF card 4-375 (Inst. of Physics, Univ. College, Cardiff, Wales)

References

- Jönsson, P. G. and Hamilton, W. C. (1970).
Acta Crystallogr. B26, 536.
Nitta, I., Sakurai, K., and Tomiie, Y. (1951).
Acta Crystallogr. 4, 289.

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C Internal standard Ag, a = 4.08651 Å | | | |
|--|----------------------------|-------|-------|
| d(Å) | I ^{rel} σ = ±5 | hkl | 1θ(°) |
| 6.15 | 10 | 1 1 0 | 14.39 |
| 4.602 | 46 | 1 0 1 | 19.27 |
| 4.130 | 100 | 2 0 0 | 21.50 |
| 4.015 | 20 | 1 2 0 | 22.12 |
| 3.768 | 10 | 2 1 0 | 23.59 |
| 3.534 | 62 | 0 2 1 | 25.18 |
| 3.312 | 1 | 2 0 1 | 26.90 |
| 3.250 | 47 | 1 2 1 | 27.42 |
| 3.116 | 43 | 2 1 1 | 28.62 |
| 3.071 | 19 | 2 2 0 | 29.05 |
| 2.769 | 12 | 0 0 2 | 32.30 |
| 2.685 | 17 | 2 2 1 | 33.34 |
| 2.650 | 6 | 0 1 2 | 33.80 |
| 2.636 | 8 | 3 1 0 | 33.98 |
| 2.625 | 9 | 1 0 2 | 34.13 |
| 2.546 | 4 | 1 3 1 | 35.22 |
| 2.525 | 10 | 1 1 2 | 35.53 |
| 2.458 | 6 | 2 3 0 | 36.53 |
| 2.381 | 7 | 3 1 1 | 37.75 |
| 2.361 | 4 | 3 2 0 | 38.09 |
| 2.295 | 3 | 0 4 0 | 39.22 |
| 2.280 | 4 | 1 2 2 | 39.50 |
| 2.246 | 2 | 2 3 1 | 40.11 |
| 2.232 | 9 | 2 1 2 | 40.38 |
| 2.211 | 13 | 1 4 0 | 40.78 |
| 2.172 | 3 | 3 2 1 | 41.54 |
| 2.119 | 1 | 0 4 1 | 42.63 |
| 2.052M | 2 | 1 4 1 | 44.09 |
| 2.052M | | 0 3 2 | 44.09 |
| 2.047 | 2 | 3 3 0 | 44.20 |
| 2.013 | 4 | 4 1 0 | 44.99 |
| 1.993 | 1 | 1 3 2 | 45.47 |
| 1.953 | 2 | 3 0 2 | 46.46 |
| 1.9100 | 14 | 3 1 2 | 47.57 |
| 1.8924 | 3 | 4 1 1 | 48.04 |
| 1.8850 | 6 | 2 4 1 | 48.24 |
| 1.8382 | 2 | 2 3 2 | 49.55 |
| 1.7955 | 1 | 3 2 2 | 50.81 |
| 1.7916 | 1 | 1 5 0 | 50.93 |
| 1.7824 | 2 | 4 2 1 | 51.21 |
| 1.7676M | 5 | 1 1 3 | 51.67 |
| 1.7676M | | 0 4 2 | 51.67 |
| 1.7622 | 7 | 3 4 0 | 51.84 |
| 1.7114 | 2 | 4 3 0 | 53.50 |
| 1.6849 | 2 | 2 0 3 | 54.41 |

Hydrazinium Sulfate, $(\text{NH}_3)_2\text{SO}_4$ - (continued)

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 5$ | hkl | $2\theta(^{\circ})$ |
|-----------------|--------------------------------------|-------|---------------------|
| 1.6778M | 2 | 2 5 0 | 54.66 |
| 1.6778M | | 1 2 3 | 54.66 |
| 1.6579 | 3 | 2 1 3 | 55.37 |
| 1.6451 | 1 | 3 3 2 | 55.84 |
| 1.6346 | 3 | 4 3 1 | 56.23 |
| 1.5821M | 2 | 5 0 1 | 58.27 |
| 1.5821M | | 2 2 3 | 58.27 |
| 1.5595 | 3 | 5 1 1 | 59.20 |

Iron Chloride Hydrate (Hydromolysite), $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$

Synonym

1. Ferric chloride hexahydrate

CAS registry no.

10025-77-1

Sample

The sample was obtained from Fisher Scientific Co., Fair Lawn, NJ. It was somewhat hygroscopic.

Color

Deep orange yellow

Structure

Monoclinic, $C2/m$ (12), $Z = 2$. The structure of $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$ was determined by Lind [1961].

Lattice constants of this sample

$a = 11.834(3) \text{ \AA}$

$b = 7.029(2)$

$c = 5.9524(13)$

$\beta = 100.47(2)^\circ$

$a/b = 1.6836$

$c/b = 0.8468$

Volume

486.8 \AA^3

Density

(calculated) 1.844 g/cm^3

Figure of merit

$F_{30} = 41.4(0.015, 47)$

Additional pattern

1. PDF card 1-153 [Hanawalt et al., 1938]

References

- Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Lind, M. D. (1967). J. Chem. Phys. 47, 990.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$ | | | | |
|---|--------------------------------------|-------|---|---|
| Internal standard Ag, $a = 4.08651 \text{ \AA}$ | | | | |
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 2$ | hkl | | |
| 6.03 | 14 | 1 | 1 | 0 |
| 5.866 | 82 | 0 | 0 | 1 |
| 5.824 | 100 | 2 | 0 | 0 |
| 4.565 | 3 | -2 | 0 | 1 |
| 4.412 | 5 | -1 | 1 | 1 |
| 4.015 | 4 | 1 | 1 | 1 |
| 3.516 | 4 | 0 | 2 | 0 |
| 3.163 | 15 | -3 | 1 | 1 |
| 3.015 | 2 | 0 | 2 | 1 |
| 2.927 | 3 | 0 | 0 | 2 |
| 2.909 | 5 | 4 | 0 | 0 |
| 2.818 | 2 | -4 | 0 | 1 |
| 2.782 | 4 | -2 | 2 | 1 |
| 2.754 | 7 | 3 | 1 | 1 |
| 2.736 | 3 | -1 | 1 | 2 |
| 2.580 | 5 | 2 | 2 | 1 |
| 2.540 | 3 | 1 | 1 | 2 |
| 2.442 | 13 | 2 | 0 | 2 |
| 2.280 | 1L | -4 | 0 | 2 |
| 2.242 | 1 | 4 | 2 | 0 |
| 2.203 | 3 | -2 | 2 | 2 |
| 2.199 | 4 | -4 | 2 | 1 |
| 2.165 | 1 | -1 | 3 | 1 |
| 2.060 | 2 | 3 | 1 | 2 |
| 2.004M | 2 | 2 | 2 | 2 |
| 2.004M | | 3 | 3 | 0 |
| 2.001 | 2 | 4 | 2 | 1 |
| 1.958 | 5 | 5 | 1 | 1 |
| 1.954 | 5 | -3 | 3 | 1 |
| 1.939 | 3 | 6 | 0 | 0 |
| 1.9096 | 3 | -1 | 1 | 3 |
| 1.8979 | 4 | 4 | 0 | 2 |
| 1.8445 | 1L | 3 | 3 | 1 |
| 1.8065 | 3 | 1 | 1 | 3 |
| 1.7721 | 2 | -6 | 0 | 2 |
| 1.7559 | 1 | 2 | 0 | 3 |
| 1.7117 | 1L | -2 | 2 | 3 |
| 1.7058M | 1 | 0 | 2 | 3 |
| 1.7058M | | -6 | 2 | 1 |
| 1.6982 | 3 | 6 | 2 | 0 |
| 1.6815 | 1L | 2 | 4 | 0 |
| 1.6702 | 1 | 4 | 2 | 2 |

Iron Fluoride Hydrate, β -FeF₃·3H₂O

Synonym

1. Ferric trifluoride trihydrate

Sample

The sample was obtained from City Chemical Corp., New York, NY.

Color

Blue gray.

Structure

Tetragonal, P4/n (85), Z = 2. The structure was determined by Teufer [1964].

Lattice constants of this sample

a = 7.8326(5) Å

c = 3.8773(3)

c/a = 0.4950

Volume

237.87 Å³

Density

(calculated) 2.330 g/cm³

Figure of merit

F₃₀ = 80.9(0.010,36)

Reference intensity

I/I_{corundum} = 2.00(4)

Polymorphism

Nielsen [1940] reported another form of FeF₃·3H₂O which was colorless and was made by crystallization at a lower temperature than the form studied here.

Additional pattern

1. PDF card 1-202 [Hanawalt et al., 1938]

References

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

Nielsen, A. H. (1940). Z. Anorg. Allgem. Chem., 244, 85.

Teufer, G. (1964). Acta Crystallogr. 17, 1480.

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C | | | | | |
|---|------------------|-----|---|---|-------|
| Internal standard W, a = 3.16524 Å | | | | | |
| d(Å) | I ^{rel} | hkl | | | 2θ(°) |
| σ = ±2 | | | | | |
| 5.542 | 100 | 1 | 1 | 0 | 15.98 |
| 3.917 | 54 | 2 | 0 | 0 | 22.68 |
| 3.879 | 14 | 0 | 0 | 1 | 22.91 |
| 3.476 | 49 | 1 | 0 | 1 | 25.61 |
| 3.177 | 25 | 1 | 1 | 1 | 28.06 |
| 2.769 | 28 | 2 | 2 | 0 | 32.30 |
| 2.600 | 10 | 2 | 1 | 1 | 34.47 |
| 2.475 | 31 | 3 | 1 | 0 | 36.27 |
| 2.253 | 1 | 2 | 2 | 1 | 39.99 |
| 2.1662 | 1L | 3 | 0 | 1 | 41.66 |
| 2.0861 | 14 | 3 | 1 | 1 | 43.34 |
| 1.9586 | 11 | 4 | 0 | 0 | 46.32 |
| 1.8950 | 13 | 3 | 2 | 1 | 47.97 |
| 1.8817 | 24 | 1 | 0 | 2 | 48.33 |
| 1.8466 | 6 | 3 | 3 | 0 | 49.31 |
| 1.8295 | 3 | 1 | 1 | 2 | 49.80 |
| 1.7512 | 26 | 4 | 2 | 0 | 52.19 |
| 1.7061 | 8 | 4 | 1 | 1 | 53.68 |
| 1.6961 | 9 | 2 | 1 | 2 | 54.02 |
| 1.6674 | 3 | 3 | 3 | 1 | 55.03 |
| 1.5962 | 3 | 4 | 2 | 1 | 57.71 |
| 1.5569 | 2 | 3 | 0 | 2 | 59.31 |
| 1.5357 | 5 | 5 | 1 | 0 | 60.21 |
| 1.5268 | 2 | 3 | 1 | 2 | 60.60 |
| 1.4524 | 3 | 4 | 3 | 1 | 64.06 |
| 1.4468 | 9 | 3 | 2 | 2 | 64.34 |
| 1.4280 | 3 | 5 | 1 | 1 | 65.29 |
| 1.3849 | 1 | 4 | 4 | 0 | 67.59 |
| 1.3620 | 4 | 5 | 2 | 1 | 68.88 |
| 1.3570 | 8 | 4 | 1 | 2 | 69.17 |
| 1.3430 | 2 | 5 | 3 | 0 | 70.00 |
| 1.3370 | 1 | 3 | 3 | 2 | 70.36 |
| 1.2920 | 1 | 0 | 0 | 3 | 73.20 |
| 1.2691 | 1 | 5 | 3 | 1 | 74.74 |
| 1.2586 | 1L | 1 | 1 | 3 | 75.47 |
| 1.2385 | 3 | 6 | 2 | 0 | 76.92 |
| 1.2275 | 1L | 2 | 0 | 3 | 77.74 |
| 1.2220 | 1 | 6 | 1 | 1 | 78.15 |
| 1.2185 | 4 | 4 | 3 | 2 | 78.42 |
| 1.2036 | 2 | 5 | 1 | 2 | 79.58 |
| 1.1712 | 1 | 2 | 2 | 3 | 82.25 |
| 1.1635 | 4 | 5 | 2 | 2 | 82.91 |
| 1.1459 | 1 | 3 | 1 | 3 | 84.48 |

Lanthanum Nickel Platinum, $\text{LaNi}_{0.25}\text{Pt}_{4.75}$

Sample

The sample was prepared at NBS by Weisman et al. [1975].

Color

Metallic gray

Structure

Hexagonal, $P6/mmm$ (191), $Z = 1$. This phase has the CaCu_5 type structure. The structure of CaCu_5 was determined by Haucke [1940].

Lattice constants of this sample

$a = 5.3732(5) \text{ \AA}$

$c = 4.3574(7)$

$c/a = 0.8110$

Volume

108.95 \AA^3

Density

(calculated) 16.465 g/cm^3

Figure of merit

$F_{20} = 69.7(0.011, 26)$

References

Haucke, W. (1940). *Z. Anorg. Allg. Chem.* **244**, 17.

Weisman, I. D., Bennett, L. H., McAlister, A. J., and Watson, R. E. (1975). *Phys. Rev. B* **11**, 82.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$ Internal standard W, $a = 3.16524 \text{ \AA}$ | | | |
|---|--------------------------------------|-------|-------------------|
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 4$ | hkl | $2\theta(^\circ)$ |
| 4.655 | 36 | 1 0 0 | 19.05 |
| 3.182 | 10 | 1 0 1 | 28.02 |
| 2.685 | 18 | 1 1 0 | 33.34 |
| 2.327 | 40 | 2 0 0 | 38.66 |
| 2.287 | 100 | 1 1 1 | 39.37 |
| 2.179 | 32 | 0 0 2 | 41.40 |
| 2.0532 | 54 | 2 0 1 | 44.07 |
| 1.9730 | 9 | 1 0 2 | 45.96 |
| 1.7591 | 5 | 2 1 0 | 51.94 |
| 1.6924 | 7 | 1 1 2 | 54.15 |
| 1.6312 | 2 | 2 1 1 | 56.36 |
| 1.5901 | 15 | 2 0 2 | 57.95 |
| 1.5512 | 4 | 3 0 0 | 59.55 |
| 1.4608 | 21 | 3 0 1 | 63.65 |
| 1.3687 | 4 | 2 1 2 | 68.50 |
| 1.3436 | 13 | 2 2 0 | 69.96 |
| 1.2774 | 8 | 1 1 3 | 74.17 |
| 1.2633 | 3 | 3 0 2 | 75.14 |
| 1.2323 | 6 | 2 0 3 | 77.38 |
| 1.1632 | 5 | 4 0 0 | 82.94 |

Lead Bromide, PbBr₂

CAS registry no.
10031-22-8

Sample

The sample originally obtained from National Lead Co. was used. These data replace a very early pattern [Swanson and Fuyat, 1953]. The new measurements have better resolution, improved intensities, and refined lattice parameters.

Major impurities

Spectrographic analysis showed 0.001 to 0.01% iron and 0.0001 to 0.001% each Ag, Al, Cu, Mg, and Si.

Color

Colorless

Structure

Orthorhombic, Pnam (62), Z = 4, isostructural with PbCl₂ [Brækken and Harang, 1928]. The structure was determined by McBride [1967].

Lattice constants of this sample

a = 8.062(1) Å
b = 9.5393(13)
c = 4.7348(6)

a/b = 0.8452
c/b = 0.4964

Volume

364.1 Å³

Density

(calculated) 6.695 g/cm³

Figure of merit

F₃₀ = 78.8(0.014,38)

Reference intensity

I/I_{corundum} = 1.83(11)

Additional patterns

1. PDF card 5-608 [Swanson and Fuyat, 1953]
2. Brækken and Harang [1928]
3. Döll and Klemm [1939]
4. Hanawalt, Rinn, and Frevel [1938]

References

- Brækken, H. and Harang, L. (1928). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 68, 123.
Döll, W. and Klemm, W. (1939). Z. Anorg. Allg. Chem. 241, 239.
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
McBride, H. D. (1967). Diss. Abstr. B27, 3891.
Swanson, H. E. and Fuyat, R. K. (1953). Nat. Bur. Stand. U.S. Circ. 539, 2, 47.

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C Internal standard W, a = 3.16524 Å | | | | |
|---|----------------------------|-------|-------|--|
| d(Å) | I ^{rel} σ = ±4 | hkl | 2θ(°) | |
| 6.16 | 3 | 1 1 0 | 14.37 | |
| 4.774 | 30 | 0 2 0 | 18.57 | |
| 4.239 | 19 | 0 1 1 | 20.94 | |
| 4.105 | 56 | 1 2 0 | 21.63 | |
| 4.032 | 31 | 2 0 0 | 22.03 | |
| 3.751 | 73 | 1 1 1 | 23.70 | |
| 3.711 | 8 | 2 1 0 | 23.96 | |
| 3.102 | 50 | 1 2 1 | 28.76 | |
| 3.081 | 55 | 2 2 0 | 28.96 | |
| 3.071 | 56 | 2 0 1 | 29.05 | |
| 2.958 | 23 | 1 3 0 | 30.19 | |
| 2.924 | 100 | 2 1 1 | 30.55 | |
| 2.641 | 90 | 0 3 1 | 33.92 | |
| 2.586 | 10 | 3 1 0 | 34.66 | |
| 2.580 | 9 | 2 2 1 | 34.74 | |
| 2.509 | 8 | 1 3 1 | 35.76 | |
| 2.495 | 15 | 2 3 0 | 35.97 | |
| 2.385 | 28 | 0 4 0 | 37.69 | |
| 2.367 | 45 | 0 0 2 | 37.98 | |
| 2.341 | 38 | 3 2 0 | 38.42 | |
| 2.286 | 14 | 1 4 0 | 39.38 | |
| 2.271 | 42 | 3 1 1 | 39.66 | |
| 2.208M | 55 | 2 3 1 | 40.83 | |
| 2.208M | | 1 1 2 | 40.83 | |
| 2.122 | 5 | 0 2 2 | 42.58 | |
| 2.099 | 4 | 3 2 1 | 43.06 | |
| 2.052M | 18 | 3 3 0 | 44.10 | |
| 2.052M | | 2 4 0 | 44.10 | |
| 2.042 | 12 | 2 0 2 | 44.32 | |
| 2.016 | 8 | 4 0 0 | 44.92 | |
| 1.997 | 2 | 2 1 2 | 45.38 | |
| 1.972 | 4 | 4 1 0 | 45.99 | |
| 1.8843M | 6 | 2 4 1 | 48.26 | |
| 1.8843M | | 3 3 1 | 48.26 | |
| 1.8773 | 11 | 2 2 2 | 48.45 | |
| 1.8568M | 4 | 4 2 0 | 49.02 | |
| 1.8568M | | 1 5 0 | 49.02 | |
| 1.8554 | 4 | 4 0 1 | 49.06 | |
| 1.8483 | 6 | 1 3 2 | 49.26 | |
| 1.7834 | 7 | 3 4 0 | 51.18 | |
| 1.7702 | 12 | 0 5 1 | 51.59 | |
| 1.7459 | 2 | 3 1 2 | 52.36 | |
| 1.7291M | 14 | 1 5 1 | 52.91 | |
| 1.7291M | | 4 2 1 | 52.91 | |
| 1.7242 | 10 | 2 5 0 | 53.07 | |
| 1.7185 | 7 | 2 3 2 | 53.26 | |
| 1.7023 | 4 | 4 3 0 | 53.81 | |
| 1.6792 | 9 | 0 4 2 | 54.61 | |
| 1.6688 | 7 | 3 4 1 | 54.98 | |
| 1.6652 | 20 | 3 2 2 | 55.11 | |

Lead Bromide, PbBr₂ - (continued)

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 4$ | hkl | $2\theta(^{\circ})$ |
|-----------------|--------------------------------------|-------|---------------------|
| 1.6448 | 4 | 1 4 2 | 55.85 |
| 1.6017 | 4 | 4 3 1 | 57.49 |
| 1.5896M | 7 | 5 1 0 | 57.97 |
| 1.5896M | | 0 6 0 | 57.97 |
| 1.5602 | 2 | 1 6 0 | 59.17 |
| 1.5564M | 3 | 0 1 3 | 59.33 |
| 1.5564M | | 3 5 0 | 59.33 |
| 1.5505M | 4 | 3 3 2 | 59.58 |
| 1.5505M | | 2 4 2 | 59.58 |
| 1.5390 | 4 | 4 4 0 | 60.07 |
| 1.5346 | 6 | 4 0 2 | 60.26 |
| 1.5295 | 7 | 1 1 3 | 60.48 |
| 1.5277 | 7 | 5 2 0 | 60.56 |
| 1.5146 | 4 | 4 1 2 | 61.14 |
| 1.5068 | 15 | 5 1 1 | 61.49 |
| 1.4793 | 20 | 2 6 0 | 62.76 |
| 1.4699 | 6 | 2 0 3 | 63.21 |
| 1.4608M | 2 | 4 2 2 | 63.65 |
| 1.4608M | | 1 5 2 | 63.65 |
| 1.4524 | 6 | 2 1 3 | 64.06 |
| 1.4384 | 1 | 5 3 0 | 64.76 |
| 1.4247 | 4 | 3 4 2 | 65.46 |
| 1.4138 | 7 | 0 3 3 | 66.03 |
| 1.4040 | 2 | 2 2 3 | 66.55 |
| 1.3938 | 2 | 2 5 2 | 67.10 |
| 1.3818 | 2 | 4 3 2 | 67.76 |
| 1.3759 | 2 | 5 3 1 | 68.09 |
| 1.3470 | 5 | 3 1 3 | 69.76 |
| 1.3358 | 7 | 5 4 0 | 70.43 |
| 1.3337 | 7 | 2 3 3 | 70.56 |
| 1.3196M | 5 | 5 1 2 | 71.43 |
| 1.3196M | | 0 6 2 | 71.43 |
| 1.3094 | 5 | 0 7 1 | 72.07 |

Lead Iodate, $\text{Pb}(\text{IO}_3)_2$

CAS registry no.
25659-31-8

Sample

The sample was made by adding solid I_2O_5 to an aqueous solution of $\text{Pb}(\text{NO}_3)_2$. This was digested by boiling for 1 hour and filtered. The solid was then heated at 300 °C for 2 hours and at 250 °C for 16 hours.

Color

Colorless

Structure

Orthorhombic, Pnaa (56), Z = 4 [Staritzky and Walker, 1956].

Lattice constants of this sample

$a = 6.090(2) \text{ \AA}$
 $b = 16.690(3)$
 $c = 5.580(2)$

$a/b = 0.3649$
 $c/b = 0.3343$

Volume

567.2 \AA^3

Density

(calculated) 6.523 g/cm^3

Figure of merit

$F_{30} = 31.1(0.017, 58)$

Reference intensity

$I/I_{\text{corundum}} = 11.9(5)$

Additional pattern

1. PDF card 11-85 [Staritzky and Walker, 1956]

Reference

Staritzky, E. and Walker, D. I. (1956). Anal. Chem. 28, 914.

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 1$ | hkl | $2\theta(^{\circ})$ |
|-----------------|--------------------------------------|--------|---------------------|
| 2.999 | 2 | 2 1 0 | 29.77 |
| 2.931 | 1 | 1 4 1 | 30.47 |
| 2.864 | 2 | 0 5 1 | 31.20 |
| 2.784 | 23 | 0 6 0 | 32.12 |
| 2.673M | 1L | 2 0 1 | 33.50 |
| 2.673M | | 2 3 0 | 33.50 |
| 2.647 | 1 | 0 2 2 | 33.84 |
| 2.594 | 4 | 1 5 1 | 34.55 |
| 2.546 | 1L | 2 2 1 | 35.22 |
| 2.508 | 1L | 1 1 2 | 35.77 |
| 2.462 | 1 | 2 4 0 | 36.47 |
| 2.307 | 1L | 1 3 2 | 39.01 |
| 2.250M | 1 | 2 5 0 | 40.04 |
| 2.250M | | 2 4 1 | 40.04 |
| 2.194 | 1L | 0 7 1 | 41.10 |
| 2.086M | 1L | 0 8 0 | 43.34 |
| 2.086M | | 2 5 1 | 43.34 |
| 2.055 | 20 | 2 6 0 | 44.04 |
| 2.043 | 6 | 2 1 2 | 44.31 |
| 1.996 | 1 | 2 2 2 | 45.39 |
| 1.969 | 11 | 0 6 2 | 46.05 |
| 1.930 | 1L | 2 3 2 | 47.05 |
| 1.895 | 1 | 3 1 1 | 47.98 |
| 1.877 | 1L | 2 7 0 | 48.47 |
| 1.860M | 3 | 3 2 1 | 48.94 |
| 1.860M | | 1 8 1 | 48.94 |
| 1.804 | 9 | 3 3 1 | 50.56 |
| 1.751 | 1 | 2 5 2 | 52.20 |
| 1.735 | 2 | 3 4 1 | 52.70 |
| 1.7215 | 1 | 2 8 0 | 53.16 |
| 1.6909 | 19 | 1 9 1 | 54.20 |
| 1.6707 | 1 | 0 8 2 | 54.91 |
| 1.6538 | 10 | 2 6 2 | 55.52 |
| 1.6373 | 1L | 1 4 3 | 56.13 |
| 1.5691 | 1L | 1 5 3 | 58.80 |
| 1.5569 | 1L | 2 7 2 | 59.31 |
| 1.5460 | 1L | 1 10 1 | 59.77 |
| 1.5220 | 1 | 4 0 0 | 60.81 |
| 1.4643+ | 1L | 0 11 1 | 63.48 |
| 1.4643+ | | 2 8 2 | 63.48 |
| 1.4235 | 1 | 1 11 1 | 65.52 |
| 1.4079 | 1 | 3 8 1 | 66.34 |
| 1.3905 | 2 | 0 12 0 | 67.28 |

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^{\circ}\text{C}$ | | | |
|---|--------------------------------------|-------|---------------------|
| Internal standard Si, $a = 5.43088 \text{ \AA}$ | | | |
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 1$ | hkl | $2\theta(^{\circ})$ |
| 8.36 | 4 | 0 2 0 | 10.57 |
| 3.996 | 2 | 1 1 1 | 22.23 |
| 3.694 | 2 | 1 2 1 | 24.07 |
| 3.309 | 100 | 1 3 1 | 26.92 |
| 3.047 | 15 | 2 0 0 | 29.29 |

Lithium Hydroxide, LiOH

CAS registry no.
1310-65-2

Sample

The sample was obtained from Fisher Scientific Co., Fair Lawn, N. J. It contained a small amount of $\text{LiOH} \cdot \text{H}_2\text{O}$ and was somewhat unstable in air. The d-spacing patterns were run with the sample in vacuum grease, and the intensity patterns run with the sample in Canada Balsam.

Structure

Tetragonal, $P4/nmm$ (129), $Z = 2$. The structure of LiOH was determined by Ernst [1933].

Lattice constants of this sample

$a = 3.5528(5) \text{ \AA}$
 $c = 4.3476(9)$

$c/a = 1.2237$

Volume
 54.88 \AA^3

Density

(calculated) 1.449 g/cm^3

Figure of merit

$F_{15} = 63.5(0.013, 18)$

Additional pattern

1. PDF card 4-708 [Ernst, 1933]

Reference

Ernst, T. (1933). Z. Phys. Chem. Leipzig
B20, 65.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$ Internal standard Si, $a = 5.43088 \text{ \AA}$ | | | |
|--|--------------------------------------|-------|-------------------|
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 2$ | hkl | $2\theta(^\circ)$ |
| 4.352 | 43 | 0 0 1 | 20.39 |
| 2.754 | 100 | 1 0 1 | 32.49 |
| 2.514 | 22 | 1 1 0 | 35.69 |
| 2.174M | 2 | 1 1 1 | 41.51 |
| 2.174M | | 0 0 2 | 41.51 |
| 1.8540 | 6 | 1 0 2 | 49.10 |
| 1.7760 | 16 | 2 0 0 | 51.41 |
| 1.6435M | 13 | 2 0 1 | 55.90 |
| 1.6435M | | 1 1 2 | 55.90 |
| 1.4919 | 10 | 2 1 1 | 62.17 |
| 1.4492 | 1 | 0 0 3 | 64.22 |
| 1.3754 | 1 | 2 0 2 | 68.12 |
| 1.3418 | 1 | 1 0 3 | 70.07 |
| 1.2828 | 3 | 2 1 2 | 73.81 |
| 1.2552 | 4 | 1 1 3 | 75.71 |
| 1.2068 | 1 | 2 2 1 | 79.33 |
| 1.1427 | 1 | 3 0 1 | 84.77 |

Magnesium Borate, MgB_4O_7

CAS registry no.
12007-62-4

Sample

The sample was prepared by heating a 1:4 molar mixture of MgCO_3 and H_3BO_3 at 600 °C for 3 days, followed by heating one hour at 800 °C, and 16 hours at 600 °C with intermittent grinding. There was a very small amount of $\text{Mg}_2\text{B}_2\text{O}_5$ present.

Color

Colorless

Structure

Orthorhombic, Pbca (61), $Z = 8$ [Kuzel, 1964].
Davis and Knight [1945] reported that this phase had the composition of MgB_2O_4 .

Lattice constants of this sample

$a = 8.596(2) \text{ \AA}$
 $b = 13.729(4)$
 $c = 7.956(2)$

$a/b = 0.6261$
 $c/b = 0.5795$

Volume
 938.9 \AA^3

Density

(calculated) 2.540 g/cm^3

Figure of merit

$F_{30} = 32.8(0.014, 64)$

Reference intensity

$I/I_{\text{corundum}} = 0.57(11)$

Additional pattern

1. PDF card 17-927 [Kuzel, 1964]

References

Davis, H. M. and Knight, M. A. (1945). J. Amer. Ceram. Soc. 28, 100.
Kuzel, H.-J. (1964). Neues Jahrb. Mineral. Monatsh. 1964, 357.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$ | | | |
|---|--------------------------------------|-------|---------------------|
| Internal standard Ag, $a = 4.08651 \text{ \AA}$ | | | |
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 2$ | hkl | $2\theta(^{\circ})$ |
| 6.86 | 21 | 0 2 0 | 12.89 |
| 5.37 | 19 | 1 1 1 | 16.50 |
| 5.196 | 98 | 0 2 1 | 17.05 |
| 4.447 | 81 | 1 2 1 | 19.95 |
| 4.098 | 24 | 2 1 0 | 21.67 |
| 3.976 | 100 | 0 0 2 | 22.34 |
| 3.636 | 37 | 2 2 0 | 24.46 |
| 3.607M | 42 | 1 0 2 | 24.66 |
| 3.607M | | 1 3 1 | 24.66 |
| 3.441 | 64 | 0 2 2 | 25.87 |
| 3.314 | 5 | 2 2 1 | 26.88 |
| 3.194 | 9 | 1 2 2 | 27.91 |
| 3.134 | 34 | 2 3 0 | 28.46 |
| 2.959 | 13 | 1 4 1 | 30.18 |
| 2.916M | 29 | 2 0 2 | 30.63 |
| 2.916M | | 2 3 1 | 30.63 |
| 2.836 | 51 | 1 3 2 | 31.52 |
| 2.683 | 33 | 2 4 0 | 33.37 |
| 2.644 | 8 | 3 1 1 | 33.87 |
| 2.542 | 6 | 2 4 1 | 35.28 |
| 2.485 | 18 | 1 5 1 | 36.12 |
| 2.474 | 21 | 0 2 3 | 36.28 |
| 2.325M | 6 | 3 0 2 | 38.70 |
| 2.325M | | 3 3 1 | 38.70 |
| 2.223M | 43 | 2 4 2 | 40.54 |
| 2.223M | | 2 5 1 | 40.54 |
| 2.203 | 11 | 3 2 2 | 40.93 |
| 2.149 | 10 | 4 0 0 | 42.01 |
| 2.123 | 2 | 4 1 0 | 42.55 |
| 2.074 | 3 | 3 3 2 | 43.61 |
| 2.051M | 5 | 4 1 1 | 44.12 |
| 2.051M | | 4 2 0 | 44.12 |
| 2.001 | 8 | 2 5 2 | 45.29 |
| 1.987M | 10 | 0 0 4 | 45.61 |
| 1.987M | | 4 2 1 | 45.61 |
| 1.958 | 7 | 2 6 1 | 46.34 |
| 1.945 | 16 | 4 3 0 | 46.67 |
| 1.924M | 21 | 3 4 2 | 47.19 |
| 1.924M | | 3 5 1 | 47.19 |
| 1.911 | 7 | 0 2 4 | 47.54 |
| 1.886 | 4 | 2 4 3 | 48.20 |
| 1.872 | 4 | 4 1 2 | 48.60 |
| 1.872 | | 3 2 3 | 48.60 |
| 1.861 | 3 | 1 5 3 | 48.89 |
| 1.822M | 7 | 4 2 2 | 50.02 |
| 1.822M | | 4 4 0 | 50.02 |
| 1.789 | 9 | 2 1 4 | 51.02 |
| 1.7450M | 5 | 2 2 4 | 52.39 |
| 1.7450M | | 3 6 1 | 52.39 |
| 1.7227 | 8 | 1 7 2 | 53.12 |

Magnesium Iodate Hydrate, $\text{Mg}(\text{IO}_3)_2 \cdot 4\text{H}_2\text{O}$

CAS registry no.
13446-17-8

Sample

The sample obtained from the Eastman Kodak Co., Rochester, NY, was recrystallized from an aqueous solution at room temperature.

Color

Colorless

Structure

Monoclinic, $P2_1/a$ (14), $Z = 2$. It was assumed to be isostructural with $\text{Co}(\text{IO}_3)_2 \cdot 4\text{H}_2\text{O}$ and $\beta\text{-Ni}(\text{IO}_3)_2 \cdot 4\text{H}_2\text{O}$ from a comparison of the powder patterns and the cell sizes. The latter compounds were studied by Abrahams et al. [1973]. Preliminary lattice constants for $\text{Mg}(\text{IO}_3)_2 \cdot 4\text{H}_2\text{O}$ were obtained by the use of the axial ratios given by Groth [1908].

Lattice constants of this sample

$a = 8.5063(15) \text{ \AA}$
 $b = 6.6362(15)$
 $c = 8.3306(12)$
 $\beta = 100.59(1)^\circ$

$a/b = 1.2818$
 $c/b = 1.2554$

Volume
 462.25 \AA^3

Density

(calculated) 3.206 g/cm^3

Figure of merit

$F_{30} = 47.8(0.015, 41)$

Reference intensity

$I/I_{\text{corundum}} = 2.44(8)$

Additional pattern

1. PDF card 20-676 [University College, Cardiff, Wales]

References

- Abrahams, S. C., Sherwood, R. C., Bernstein, J. L., and Nassau, K. (1973). *J. Solid State Chem.* 7, 205.
Groth, P. (1908). *Chemische Krystallographie II* (Engelmann, Leipzig, Germany) p. 120.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$ | | | |
|---|--------------------------------------|--------|-------------------|
| Internal standard Si, $a = 5.43088 \text{ \AA}$ | | | |
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 2$ | hkl | $2\theta(^\circ)$ |
| 8.18 | 24 | 0 0 1 | 10.81 |
| 5.154 | 100 | 0 1 1 | 17.19 |
| 4.631 | 13 | -1 1 1 | 19.15 |
| 4.174M | 74 | 2 0 0 | 21.27 |
| 4.174M | | 1 1 1 | 21.27 |
| 4.094 | 12 | 0 0 2 | 21.69 |
| 3.535 | 8 | 2 1 0 | 25.17 |
| 3.478 | 55 | 2 0 1 | 25.59 |
| 3.445 | 48 | -2 1 1 | 25.84 |
| 3.413 | 8 | -1 1 2 | 26.09 |
| 3.318 | 5 | 0 2 0 | 26.85 |
| 3.236 | 13 | -2 0 2 | 27.54 |
| 3.077M | 15 | 2 1 1 | 29.00 |
| 3.077M | | 0 2 1 | 29.00 |
| 3.052 | 2 | 1 1 2 | 29.24 |
| 2.954 | 30 | -1 2 1 | 30.23 |
| 2.912 | 4 | -2 1 2 | 30.68 |
| 2.826 | 4 | 1 2 1 | 31.64 |
| 2.728 | 22 | 0 0 3 | 32.80 |
| 2.599 | 9 | 2 2 0 | 34.48 |
| 2.577M | 6 | -3 1 1 | 34.78 |
| 2.577M | | 0 2 2 | 34.78 |
| 2.570 | 6 | 3 1 0 | 34.88 |
| 2.540 | 9 | -1 1 3 | 35.31 |
| 2.525 | 5 | 0 1 3 | 35.52 |
| 2.506 | 5 | -2 0 3 | 35.81 |
| 2.493 | 6 | 2 1 2 | 36.00 |
| 2.397 | 6 | 2 2 1 | 37.49 |
| 2.387 | 11 | 1 2 2 | 37.66 |
| 2.364 | 3 | -3 1 2 | 38.04 |
| 2.343M | 2 | -2 1 3 | 38.39 |
| 2.343M | | 3 1 1 | 38.39 |
| 2.316 | 4 | -2 2 2 | 38.85 |
| 2.311 | 3 | 1 1 3 | 38.94 |
| 2.137M | 17 | 1 3 0 | 42.26 |
| 2.137M | | 0 3 1 | 42.26 |
| 2.114 | 6 | 2 0 3 | 42.74 |
| 2.089M | 4 | 4 0 0 | 43.27 |
| 2.089M | | 2 2 2 | 43.27 |
| 2.046M | 4 | 0 0 4 | 44.23 |
| 2.046M | | 1 3 1 | 44.23 |
| 2.019M | 11 | -4 1 1 | 44.85 |
| 2.019M | | -4 0 2 | 44.85 |
| 2.015 | 11 | 2 1 3 | 44.95 |
| 1.994 | 4 | 4 1 0 | 45.46 |
| 1.956M | 4 | 0 1 4 | 46.39 |
| 1.956M | | 2 3 0 | 46.39 |
| 1.941M | 4 | 4 0 1 | 46.76 |
| 1.941M | | -2 3 1 | 46.76 |
| 1.904 | 5 | -2 1 4 | 47.72 |

Magnesium Iodate Hydrate, $\text{Mg}(\text{IO}_3)_2 \cdot 4\text{H}_2\text{O}$ - (continued)

| $d(\text{\AA})$ | I^{rel} $\sigma \approx \pm 2$ | hkl | $2\theta(^{\circ})$ |
|-----------------|--|--------|---------------------|
| 1.866 | 1 | 2 3 1 | 48.77 |
| 1.834 | 3 | 1 1 4 | 49.68 |
| 1.7925 | 2 | 3 2 2 | 50.90 |
| 1.7619 | 3 | -1 2 4 | 51.85 |
| 1.7425 | 2 | 0 2 4 | 52.47 |
| 1.7370 | 4 | 4 0 2 | 52.65 |
| 1.7327 | 4 | 3 3 0 | 52.79 |
| 1.7236M | 7 | -4 2 2 | 53.09 |
| 1.7236M | | -1 3 3 | 53.09 |
| 1.6801 | 2 | 4 1 2 | 54.58 |
| 1.6758 | 2 | 4 2 1 | 54.73 |
| 1.6654 | 2 | -3 3 2 | 55.10 |
| 1.6465 | 2 | 1 3 3 | 55.79 |
| 1.6298 | 1 | -2 0 5 | 56.41 |
| 1.6190 | 1 | -4 0 4 | 56.82 |
| 1.6092 | 2 | -5 1 2 | 57.20 |
| 1.5901 | 4 | 0 1 5 | 57.95 |
| 1.5730 | 2 | -4 1 4 | 58.64 |

α -Manganese, Mn

CAS registry no.

7439-96-5

Sample

The sample was obtained from Fisher Scientific Co., Fair Lawn, NJ. It was annealed in vacuum at 650 °C for 4 hours.

Color

Metallic gray

Structure

Cubic, $\overline{14}3m$ (217), $Z = 58$ [Gazzara et al., 1967].

Lattice constant of this sample

$a = 8.9121$ (4) Å

Volume

707.85 Å³

Density

(calculated) 7.475 g/cm³

Figure of merit

$F_{30} = 69.9$ (0.012,37)

Polymorphism

There are also β , γ , and δ Mn, the most probable transition temperatures being $\alpha \rightleftharpoons \beta$, 700 °C; $\beta \rightleftharpoons \gamma$, 1079 °C; $\alpha \rightleftharpoons \delta$ 1143 °C [Sully, 1955].

Additional patterns

1. PDF card 1-1237 [Hanawalt et al., 1938].
2. PDF card 20-180 [Swanson et al., 1969].

References

- Gazzara, C. P., Middleton, R. M., Weiss, R. J., and Hall, E. O. (1967). Acta Crystallogr. 22, 859.
- Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
- Sully, A. H. (1955). Manganese (Butterworth Scientific Publications, London), p. 127.
- Swanson, H. E., McMurdie, H. F., Morris, M. C., and Evans, E. H. (1969). Nat'l. Bur. Std. U.S. Monogr. 25, Sec. 7, 142.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. 25 \pm 1 $^{\circ}\text{C}$ | | | | |
|---|--------------------------------------|-----|-----|---------------------|
| Internal standard W, $a = 3.16524 \text{ \AA}$ | | | | |
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 2$ | hkl | | $2\theta(^{\circ})$ |
| 3.641 | 1L | 2 | 1 1 | 24.43 |
| 3.153 | 1 | 2 | 2 0 | 28.28 |
| 2.571 | 3 | 2 | 2 2 | 34.87 |
| 2.382 | 3 | 3 | 2 1 | 37.74 |
| 2.227 | 7 | 4 | 0 0 | 40.48 |
| 2.101 | 100 | 4 | 1 1 | 43.01 |
| 1.8994 | 24 | 3 | 3 2 | 47.85 |
| 1.8193 | 9 | 4 | 2 2 | 50.10 |
| 1.7475 | 14 | 5 | 1 0 | 52.31 |
| 1.6274 | 1 | 5 | 2 1 | 56.50 |
| 1.5286 | 1L | 5 | 3 0 | 60.52 |
| 1.4857 | 1 | 6 | 0 0 | 62.46 |
| 1.4460 | 1 | 6 | 1 1 | 64.38 |
| 1.4088 | 1L | 6 | 2 0 | 66.29 |
| 1.3754 | 1L | 5 | 4 1 | 68.12 |
| 1.3435 | 2 | 6 | 2 2 | 69.97 |
| 1.3138 | 1L | 6 | 3 1 | 71.79 |
| 1.2864 | 4 | 4 | 4 4 | 73.57 |
| 1.2605 | 7 | 7 | 1 0 | 75.34 |
| 1.2125 | 17 | 7 | 2 1 | 78.88 |
| 1.1911 | 3 | 6 | 4 2 | 80.59 |
| 1.1701 | 2 | 7 | 3 0 | 82.34 |
| 1.1317 | 3 | 7 | 3 2 | 85.79 |
| 1.0969 | 2 | 8 | 1 1 | 89.22 |
| 1.0806 | 1 | 8 | 2 0 | 90.93 |
| 1.0652 | 1 | 6 | 5 3 | 92.63 |
| 1.0504 | 6 | 8 | 2 2 | 94.33 |
| 1.0361 | 1 | 8 | 3 1 | 96.05 |
| 1.0223 | 1L | 6 | 6 2 | 97.79 |
| 1.0091 | 1 | 7 | 5 2 | 99.52 |

Mercury Acetate, $C_4H_6Hg_2O_4$

Synonym

1. Mercurous Acetate

CAS registry no.

631-60-7

Sample

$Hg_2(NO_3)_2 \cdot 2H_2O$ was dissolved in water with addition of 25% HNO_3 and treated with a solution of CH_3CO_2Na . The precipitate was washed with cold water and dried in a desiccator [Brauer, 1963].

Color

Colorless

Structure

Monoclinic, $A^*/*$, $Z = 2$ [Puff et al., 1965].

Lattice constants of this sample

$a = 12.185(3) \text{ \AA}$

$b = 5.966(2)$

$c = 5.1867(13)$

$\beta = 100.08(2)^\circ$

$a/b = 2.0424$

$c/b = 0.8694$

Volume

371.2 \AA^3

Density

(calculated) 4.645 g/cm^3

Figure of merit

$F_{30} = 54.5(0.013, 42)$

Additional pattern

1. PDF card 19-799 [Puff et al., 1965]

References

Brauer, G. (1963). Handbook of Preparative Inorganic Chemistry, (Academic Press, New York, NY) p. 1120.

Puff, H., Lorbacher, G., and Skrabs, R. (1965). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 122, 156.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$ | | | |
|---|--------------------------------------|--------|-------------------|
| Internal standard Ag, $a = 4.08651 \text{ \AA}$ | | | |
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 2$ | hkl | $2\theta(^\circ)$ |
| 12.02 | 100 | 1 0 0 | 7.35 |
| 6.00 | 1 | 2 0 0 | 14.74 |
| 4.001 | 3 | 3 0 0 | 22.20 |
| 3.877 | 11 | 0 1 1 | 22.92 |
| 3.849 | 15 | -1 1 1 | 23.09 |
| 3.553 | 2 | 1 1 1 | 25.04 |
| 3.477 | 14 | -2 1 1 | 25.60 |
| 3.079 | 1 | 2 1 1 | 28.98 |
| 3.000 | 14 | 4 0 0 | 29.76 |
| 2.894 | 5 | 1 2 0 | 30.87 |
| 2.615 | 4 | 3 1 1 | 34.26 |
| 2.593 | 2 | -1 0 2 | 34.57 |
| 2.544 | 1L | -4 1 1 | 35.25 |
| 2.514 | 3 | -2 0 2 | 35.69 |
| 2.399 | 8 | 5 0 0 | 37.46 |
| 2.346 | 2 | -3 0 2 | 38.33 |
| 2.233 | 8 | 4 1 1 | 40.35 |
| 2.215 | 2 | 2 0 2 | 40.71 |
| 2.174 | 2 | -5 1 1 | 41.51 |
| 2.137 | 1 | -4 0 2 | 42.26 |
| 2.115 | 3 | 4 2 0 | 42.72 |
| 2.000M | 6 | 6 0 0 | 45.30 |
| 2.000M | | 3 0 2 | 45.30 |
| 1.956 | 1 | -1 2 2 | 46.39 |
| 1.928 | 3 | 5 1 1 | 47.10 |
| 1.924 | 3 | -5 0 2 | 47.20 |
| 1.882 | 4 | -6 1 1 | 48.32 |
| 1.870 | 3 | 5 2 0 | 48.64 |
| 1.849 | 2 | -1 3 1 | 49.23 |
| 1.845 | 2 | -3 2 2 | 49.36 |
| 1.8031 | 1 | -2 3 1 | 50.58 |
| 1.7958 | 1 | 4 0 2 | 50.80 |
| 1.7769 | 1 | 2 2 2 | 51.38 |
| 1.7276 | 1L | -6 0 2 | 52.96 |
| 1.7141 | 1L | 7 0 0 | 53.41 |
| 1.6602+ | 2 | -1 1 3 | 55.29 |
| 1.6602+ | | 3 2 2 | 55.29 |
| 1.6503M | 2 | -7 1 1 | 55.65 |
| 1.6503M | | -2 1 3 | 55.65 |

Mercury Hydroxide Nitrate, $\text{Hg}(\text{OH})\text{NO}_3$

Synonym

1. Mercury oxide nitrate hydrate,
 $\text{Hg}_2\text{O}(\text{NO}_3)_2 \cdot \text{H}_2\text{O}$

Sample

The sample was prepared by dissolving $\text{HgNO}_3 \cdot \text{H}_2\text{O}$ in a mixture of HNO_3 and H_2O . The solution was evaporated at room temperature. The first crystals formed were a mixture of phases and were discarded. The second crystals formed were used to obtain the measurements.

Color

Colorless

Structure

Monoclinic, $P2_1/n$ (14), $Z = 4$. The structure was determined by Ribár et al. [1971].

Lattice constants of this sample

$a = 7.7438(11) \text{ \AA}$
 $b = 7.1944(11)$
 $c = 6.5893(11)$
 $\beta = 114.28(1)^\circ$

$a/b = 1.0764$
 $c/b = 0.9159$

Volume

334.62 \AA^3

Density

(calculated) 5.550 g/cm^3

Figure of merit

$F_{30} = 39.1 (0.013, 58)$

Reference intensity

$I/I_{\text{corundum}} = 9.2(5)$

Additional pattern

1. PDF card 11-189 [Bernstein et al., 1957]

References

Bernstein, R. B., Pars, H. G., and Blumenthal, D. C. (1957). J. Am. Chem. Soc. **79**, 1579.
 Ribár, B., Matković, B., Sljukić, M., and Gabela, F. (1971). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. **134**, 311.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$ | | | | |
|---|--------------------------------------|-----|---|---|
| Internal standard Ag, $a = 4.08651 \text{ \AA}$ | | | | |
| $d(\text{Å})$ | I^{rel} $\sigma = \pm 2$ | hkl | | |
| 5.93 | 100 | -1 | 0 | 1 |
| 4.614 | 1 | 0 | 1 | 1 |
| 4.583 | 2 | -1 | 1 | 1 |
| 3.862 | 33 | 1 | 0 | 1 |
| 3.526 | 18 | 2 | 0 | 0 |
| 3.404 | 2 | 1 | 1 | 1 |
| 3.361 | 2 | -2 | 1 | 1 |
| 3.207 | 32 | 1 | 2 | 0 |
| 3.088 | 18 | 0 | 2 | 1 |
| 3.005 | 19 | 0 | 0 | 2 |
| 2.969 | 19 | -2 | 0 | 2 |
| 2.630 | 3 | 1 | 2 | 1 |
| 2.612 | 12 | -2 | 2 | 1 |
| 2.582 | 9 | -3 | 0 | 1 |
| 2.454 | 3 | 2 | 1 | 1 |
| 2.430M | 11 | -1 | 2 | 2 |
| 2.430M | | -3 | 1 | 1 |
| 2.267 | 1 | -3 | 1 | 2 |
| 2.236 | 1L | 3 | 1 | 0 |
| 2.176 | 6 | -1 | 0 | 3 |
| 2.113 | 5 | 2 | 2 | 1 |
| 2.012 | 4 | 1 | 2 | 2 |
| 1.991 | 5 | -3 | 2 | 2 |
| 1.984 | 4 | 2 | 3 | 0 |
| 1.979 | 4 | -3 | 0 | 3 |
| 1.970 | 4 | 3 | 2 | 0 |
| 1.937 | 1 | 3 | 0 | 1 |
| 1.930M | 2 | 2 | 0 | 2 |
| 1.930M | | 0 | 1 | 3 |
| 1.9013 | 2 | -4 | 0 | 2 |
| 1.8704 | 1 | 3 | 1 | 1 |
| 1.8547M | 4 | -4 | 1 | 1 |
| 1.8547M | | -2 | 2 | 3 |
| 1.8378 | 1L | -4 | 1 | 2 |
| 1.7982 | 3 | 0 | 4 | 0 |
| 1.7641 | 1 | 4 | 0 | 0 |
| 1.7487 | 3 | 0 | 2 | 3 |
| 1.7435 | 2 | 1 | 4 | 0 |
| 1.7206 | 3 | -1 | 4 | 1 |
| 1.7135 | 1 | 4 | 1 | 0 |
| 1.6938M | 2 | -4 | 2 | 1 |
| 1.6938M | | -3 | 3 | 2 |
| 1.6470 | 1 | -2 | 0 | 4 |
| 1.6298 | 2 | 1 | 4 | 1 |
| 1.6266 | 1 | -2 | 4 | 1 |

Mercury Hydroxide Nitrate, $\text{Hg}(\text{OH})\text{NO}_3$ - (continued)

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 2$ | hkl | $2\theta(^{\circ})$ |
|-----------------|--------------------------------------|--------|---------------------|
| 1.6025 | 1 | 2 4 0 | 57.46 |
| 1.5519 | 1 | -4 2 3 | 59.52 |
| 1.5425 | 2 | 0 4 2 | 59.92 |
| 1.5383 | 2 | -2 4 2 | 60.10 |
| 1.5204 | 1L | -5 0 1 | 60.88 |
| 1.5013 | 1 | 0 0 4 | 61.74 |
| 1.4978M | 1L | 4 1 1 | 61.90 |
| 1.4978M | | -2 2 4 | 61.90 |
| 1.4874 | 1 | -5 1 1 | 62.38 |
| 1.4836 | 1 | -4 0 4 | 62.56 |
| 1.4743 | 1 | -5 0 3 | 63.00 |
| 1.4699M | 2 | 0 1 4 | 63.21 |
| 1.4699M | | -1 2 4 | 63.21 |
| 1.4608 | 1 | -3 2 4 | 63.65 |

Niobium Boride, ζ -NbB

CAS registry no.
12045-19-1

Sample

The sample obtained from the metallurgy Section at NBS was a mixture of ζ -NbB + Nb.

Color

Metallic gray

Structure

Orthorhombic, Cmc \bar{m} (63), Z = 4. The structure was studied by Andersson and Kiessling [1950] and by Brewer et al., [1951]. It is isostructural with CrB.

Lattice constants of this sample

$a = 3.2973(4) \text{ \AA}$
 $b = 8.7229(10)$
 $c = 3.1663(3)$

$a/b = 0.3780$
 $c/b = 0.3630$

Volume
 91.069 \AA^3

Density

(calculated) 7.565 g/cm^3

Figure of merit

$F_{27} = 74.4(0.0095, 38)$

Additional pattern

1. PDF card 29-947 [Spear, K. and Blanks, Pennsylvania State University, University Park, PA].

References

- Andersson, L. H. and Kiessling, R. (1950). Acta Chem. Scand. 4, 160.
Brewer, L., Sawyer, D. L., Templeton, D. H., and Dauben, C. H. (1951). J. Amer. Ceram. Soc. 34, No. 6, 173.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$ Internal standard Si, $a = 5.43088 \text{ \AA}$ | | | |
|--|--------------------------------------|-------|-------------------|
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 4$ | hkl | $2\theta(^\circ)$ |
| 4.363 | 7 | 0 2 0 | 20.34 |
| 3.084 | 46 | 1 1 0 | 28.93 |
| 2.564 | 80 | 0 2 1 | 34.97 |
| 2.209 | 100 | 1 1 1 | 40.81 |
| 2.181M | 97 | 1 3 0 | 41.37 |
| 2.181M | | 0 4 0 | 41.37 |
| 1.7965M | 30 | 1 3 1 | 50.78 |
| 1.7965M | | 0 4 1 | 50.78 |
| 1.6481 | 18 | 2 0 0 | 55.73 |
| 1.5831 | 13 | 0 0 2 | 58.23 |
| 1.5418M | 2 | 2 2 0 | 59.95 |
| 1.5418M | | 1 5 0 | 59.95 |
| 1.4885 | 1 | 0 2 2 | 62.33 |
| 1.4540 | 6 | 0 6 0 | 63.98 |
| 1.4087 | 10 | 1 1 2 | 66.30 |
| 1.3863M | 52 | 2 2 1 | 67.51 |
| 1.3863M | | 1 5 1 | 67.51 |
| 1.3212 | 8 | 0 6 1 | 71.33 |
| 1.3148 | 10 | 2 4 0 | 71.73 |
| 1.2808M | 27 | 1 3 2 | 73.94 |
| 1.2808M | | 0 4 2 | 73.94 |
| 1.2145 | 6 | 2 4 1 | 78.73 |
| 1.1656 | 14 | 1 7 0 | 82.73 |
| 1.1419 | 9 | 2 0 2 | 84.84 |
| 1.1047M | 2 | 2 2 2 | 88.42 |
| 1.1047M | | 1 5 2 | 88.42 |
| 1.0904+ | 5 | 2 6 0 | 89.89 |
| 1.0904+ | | 0 8 0 | 89.89 |
| 1.0707 | 3 | 0 6 2 | 92.01 |
| 1.0308+ | 17 | 2 6 1 | 96.71 |
| 1.0308+ | | 0 8 1 | 96.71 |
| 1.0283 | 13 | 3 3 0 | 97.03 |
| 1.0257 | 7 | 0 2 3 | 97.35 |
| 1.0116 | 8 | 2 4 2 | 99.18 |
| .9986 | 6 | 1 1 3 | 100.96 |

Pentaerythritol, C₅H₁₂O₄

Synonym

1. 2,2-Bis(hydroxymethyl)-1,3-propanediol

CAS registry no.

115-77-5

Sample

The sample was obtained from Eastman Organic Chemicals, Rochester, NY. It was recrystallized from ethanol.

Color

Colorless

Structure

Tetragonal, $I\bar{4}$ (82), $Z = 2$. The structure was determined by Llewellyn et al. [1937] and Nitta and Watanabé [1937] and [1938a]. It was later refined by Shiono et al. [1957], [1958].

Lattice constants of this sample

$$a = 6.0890(12) \text{ \AA}$$

$$c = 8.7481(16)$$

$$c/a = 1.4367$$

Volume

$$324.34 \text{ \AA}^3$$

Density

$$(\text{calculated}) 1.394 \text{ g/cm}^3$$

Figure of merit

$$F_{23} = 58.9(0.012, 33)$$

Reference intensity

$$I/I_{\text{corundum}} = 5.33(7)$$

Polymorphism

There is a cubic high temperature form stable from 179.5 °C to the melting point (260.5 °C). [Nitta and Watanabé, 1938b].

Additional pattern

1. PDF card 3-214 [Dow Chemical Co. Midland, MI]

References

- Llewellyn, F. J., Cox, E. G., and Goodwin, T. H. (1937). J. Chem. Soc. London, 1937, 883.
- Nitta, I. and Watanabé, T. (1937). Nature London 140, 365.
- Nitta, I. and Watanabé, T. (1938a). Sci. Pap. Inst. Phys. Chem. Res. Tokyo 34, 1669.
- Nitta, I. and Watanabé, T. (1938b). Bull. Chem. Soc. Japan 13, 28.
- Shiono, R., Cruickshank, D. W. J., and Cox, E. G. (1957). Acta Crystallogr. 10, 794.
- Shiono, R., Cruickshank, D. W. J., and Cox, E. G. (1958). Acta Crystallogr. 11, 387.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$ Internal standard W, $a = 3.16524 \text{ \AA}$ | | | |
|---|------------------------------------|-------|-------------------|
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm$ | hkl | $2\theta(^\circ)$ |
| 4.998 | 6 | 1 0 1 | 17.73 |
| 4.371 | 100 | 0 0 2 | 20.30 |
| 4.306 | 4 | 1 1 0 | 20.61 |
| 3.068 | 7 | 1 1 2 | 29.08 |
| 3.044 | 4 | 2 0 0 | 29.32 |
| 2.632 | 2 | 1 0 3 | 34.04 |
| 2.601 | 4 | 2 1 1 | 34.46 |
| 2.499 | 3 | 2 0 2 | 35.90 |
| 2.186 | 1 | 0 0 4 | 41.26 |
| 2.153 | 1 | 2 2 0 | 41.93 |
| 1.991 | 2 | 2 1 3 | 45.53 |
| 1.9506 | 1 | 1 1 4 | 46.52 |
| 1.9314 | 2 | 2 2 2 | 47.01 |
| 1.7769 | 1L | 2 0 4 | 51.38 |
| 1.7619 | 1L | 3 1 2 | 51.85 |
| 1.6815 | 1L | 1 0 5 | 54.53 |
| 1.6649 | 1 | 3 0 3 | 55.12 |
| 1.6591 | 1 | 3 2 1 | 55.33 |
| 1.5336 | 1L | 2 2 4 | 60.30 |
| 1.4722 | 1L | 2 1 5 | 63.10 |
| 1.4581 | 1L | 0 0 6 | 63.78 |
| 1.4451 | 1L | 3 1 4 | 64.42 |
| 1.3250 | 1L | 3 0 5 | 71.09 |

Phenylhydrazine Hydrochloride, $C_6H_8N_2 \cdot HCl$

Synonym

1. Hydrazinobenzene hydrochloride

CAS registry no.

59-88-1

Sample

The sample was obtained from Eastman Kodak Co., Rochester, NY. One of the lines at $2\theta = 38.96^\circ$ came only within 0.06° of the calculated value.

Color

Colorless

Structure

Monoclinic, $P2_1/n$ (14), $Z = 4$. The structure was studied by Koo [1965].

Lattice constants of this sample

$a = 6.066(2) \text{ \AA}$

$b = 30.641(6)$

$c = 3.884(2)$

$\beta = 100.86(5)^\circ$

$a/b = 0.1980$

$c/b = 0.1268$

Volume

709.0 \AA^3

Density

(calculated) 1.355 g/cm^3

Figure of merit

$F_{30} = 13.0(0.014, 172)$

Reference intensity

$I/I_{\text{corundum}} = 1.28(14)$

Reference

Koo, O. H. (1965). Bull. Chem. Soc. Jpn. 38, 262.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$ Internal standard W, $a = 3.16524 \text{ \AA}$ | | | |
|---|--------------------------------------|---------|-------------------|
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 3$ | hkl | $2\theta(^\circ)$ |
| 15.30 | 100 | 0 2 0 | 5.77 |
| 7.66 | 22 | 0 4 0 | 11.54 |
| 5.556 | 30 | 1 2 0 | 15.94 |
| 4.706 | 22 | 1 4 0 | 18.84 |
| 3.831 | 90 | 0 8 0 | 23.20 |
| 3.700 | 20 | 0 2 1 | 24.03 |
| 3.524M | 8 | -1 0 1 | 25.25 |
| 3.524M | | 1 7 0 | 25.25 |
| 3.507 | 12 | -1 1 1 | 25.38 |
| 3.417 | 22 | 0 4 1 | 26.06 |
| 3.224 | 13 | 1 8 0 | 27.65 |
| 3.065 | 33 | 0 10 0 | 29.11 |
| 2.977 | 41 | 2 0 0 | 29.99 |
| 2.924 | 12 | 2 2 0 | 30.55 |
| 2.901 | 4 | -1 6 1 | 30.80 |
| 2.703 | 4 | 0 8 1 | 33.11 |
| 2.555 | 33 | 0 12 0 | 35.09 |
| 2.352 | 8 | 2 8 0 | 38.24 |
| 2.310 | 4 | -1 10 1 | 38.96 |
| 2.188 | 1 | 0 14 0 | 41.22 |
| 2.185 | 2 | -1 11 1 | 41.28 |
| 2.137M | 9 | 2 2 1 | 42.26 |
| 2.137M | | 2 10 0 | 42.26 |
| 2.065 | 3 | -2 9 1 | 43.81 |
| 2.034 | 1 | 2 11 0 | 44.51 |
| 1.938 | 8 | 2 12 0 | 46.83 |
| 1.9160M | 3 | -3 0 1 | 47.41 |
| 1.9160M | | 0 16 0 | 47.41 |
| 1.8234M | 5 | 1 16 0 | 49.98 |
| 1.8234M | | 2 9 1 | 49.98 |
| 1.7616+ | 2 | -1 7 2 | 51.86 |
| 1.7616+ | | 1 14 1 | 51.86 |
| 1.7111 | 5 | 0 16 1 | 53.51 |
| 1.6696 | 1 | -3 9 1 | 54.95 |
| 1.6370+ | 2 | 3 1 1 | 56.14 |
| 1.6370+ | | 1 18 0 | 56.14 |
| 1.6105 | 1 | 2 16 0 | 57.15 |
| 1.6061M | 1 | -2 15 1 | 57.32 |
| 1.6061M | | -1 17 1 | 57.32 |
| 1.5545 | 1 | 0 18 1 | 59.41 |
| 1.5323M | 2 | -3 12 1 | 60.36 |
| 1.5323M | | 0 20 0 | 60.36 |
| 1.4823M | 2 | 4 2 0 | 62.62 |
| 1.4823M | | -3 5 2 | 62.62 |
| 1.4778+ | 2 | -4 2 1 | 62.83 |
| 1.4778+ | | 2 18 0 | 62.83 |

Potassium Arsenic Fluoride, KAsF_6

Synonym

1. Potassium hexafluoroarsenate

CAS registry no.

17029-22-0

Sample

The sample was obtained from Alfa Inorganics, Beverly, MA.

Color

Colorless

Structure

Hexagonal, $R\bar{3}m$ (166), $Z = 3$. The structure was determined by Roof [1955] and refined by Ibers [1956]. It is isostructural with NH_4SbF_6 .

Lattice constants of this sample

$a = 7.3780(4) \text{ \AA}$

$c = 7.3095(5)$

$c/a = 0.9907$

Volume

344.58 \AA^3

Density

(calculated) 3.296 g/cm^3

Figure of merit

$F_{30} = 100.6(0.009, 32)$

Reference intensity

$I/I_{\text{corundum}} = 3.00(8)$

References

Roof, R. B. Jr., (1955). Acta Crystallogr. 8, 739.

Ibers, J. A. (1956). Acta Crystallogr. 9, 967.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$ Internal standard W, $a = 3.16524 \text{ \AA}$ | | | | | |
|---|--------------------------------------|-----|---|---|-------------------|
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 2$ | hkl | | | $2\theta(^\circ)$ |
| 4.810 | 69 | 1 | 0 | 1 | 18.43 |
| 3.684 | 100 | 1 | 1 | 0 | 24.14 |
| 3.170 | 62 | 0 | 1 | 2 | 28.13 |
| 2.927 | 14 | 0 | 2 | 1 | 30.52 |
| 2.436 | 3 | 0 | 0 | 3 | 36.87 |
| 2.405 | 7 | 2 | 0 | 2 | 37.36 |
| 2.293 | 4 | 2 | 1 | 1 | 39.26 |
| 2.1287 | 5 | 3 | 0 | 0 | 42.43 |
| 2.0317 | 7 | 1 | 1 | 3 | 44.56 |
| 2.0146 | 50 | 1 | 2 | 2 | 44.96 |
| 1.8445 | 7 | 2 | 2 | 0 | 49.37 |
| 1.7569 | 2 | 1 | 0 | 4 | 52.01 |
| 1.7227 | 5 | 1 | 3 | 1 | 53.12 |
| 1.6035 | 5 | 3 | 0 | 3 | 57.42 |
| 1.5947 | 5 | 3 | 1 | 2 | 57.77 |
| 1.5859 | 6 | 0 | 2 | 4 | 58.12 |
| 1.4707 | 3 | 2 | 2 | 3 | 63.17 |
| 1.4632 | 9 | 0 | 4 | 2 | 63.53 |
| 1.4571 | 12 | 2 | 1 | 4 | 63.83 |
| 1.4370 | 2 | 3 | 2 | 1 | 64.83 |
| 1.3943 | 6 | 4 | 1 | 0 | 67.07 |
| 1.3605 | 4 | 2 | 3 | 2 | 68.97 |
| 1.3293 | 1 | 2 | 0 | 5 | 70.83 |
| 1.2720 | 2 | 1 | 3 | 4 | 74.54 |
| 1.2588 | 1L | 0 | 5 | 1 | 75.46 |
| 1.2506 | 1L | 1 | 2 | 5 | 76.04 |
| 1.2299 | 3 | 3 | 3 | 0 | 77.56 |
| 1.2181 | 1 | 0 | 0 | 6 | 78.45 |
| 1.2101 | 1 | 4 | 1 | 3 | 79.07 |
| 1.2063 | 3 | 5 | 0 | 2 | 79.37 |
| 1.2028 | 3 | 4 | 0 | 4 | 79.65 |
| 1.1914 | 1 | 2 | 4 | 1 | 80.56 |
| 1.1570 | 2 | 1 | 1 | 6 | 83.48 |
| 1.1466 | 2 | 4 | 2 | 2 | 84.41 |
| 1.1436 | 2 | 3 | 2 | 4 | 84.69 |
| 1.1338 | 1 | 5 | 1 | 1 | 85.59 |
| 1.1279 | 1 | 3 | 1 | 5 | 86.15 |
| 1.0951 | 1L | 1 | 5 | 2 | 89.40 |
| 1.0649 | 1L | 6 | 0 | 0 | 92.66 |
| 1.0574 | 1 | 3 | 0 | 6 | 93.52 |
| 1.0473 | 1L | 0 | 5 | 4 | 94.70 |
| 1.0398 | 1 | 4 | 3 | 1 | 95.60 |
| 1.0352 | 1L | 2 | 3 | 5 | 96.16 |
| 1.0307 | 1L | 1 | 0 | 7 | 96.73 |
| 1.0231 | 1L | 5 | 2 | 0 | 97.69 |
| 1.0165 | 1L | 2 | 2 | 6 | 98.54 |
| 1.0093 | 1L | 3 | 4 | 2 | 99.49 |
| 1.0074 | 1L | 2 | 4 | 4 | 99.75 |

Potassium Hydrogen Iodate, γ -KH(IO₃)₂

CAS registry no.
13455-24-8

Sample

A sample labelled KH(IO₃)₂ was obtained from Fisher Scientific Co., Fair Lawn, N. J. It was recrystallized in water solution with the pH adjusted with I₂O₅. This γ -phase decomposes in moist air and minor amounts of another phase may be present. The reflection, $d = 4.590$ and $I = 15$ has $|2\theta_{\text{obs}} - 2\theta_{\text{calc}}| = 0.056^\circ$.

Color

Colorless

Structure

Monoclinic, $P2_1/c$ (14), $Z = 8$ [Argay et al., 1969].

Lattice constants of this sample

$a = 21.853(5) \text{ \AA}$
 $b = 8.206(3)$
 $c = 7.031(2)$
 $\beta = 98.02(3)^\circ$

$a/b = 2.6631$
 $c/b = 0.8568$

Volume \AA^3
1249.

Density

(calculated) 4.149 g/cm^3

Figure of merit

$F_{30} = 16.8(0.018, 97)$

Polymorphism

The monoclinic polymorph, α -KH(IO₃)₂, also has the space group $P2_1/a$ but a cell volume of 629.6 \AA^3 [Argay et al., 1969].

Additional pattern

1. Argay et al. [1969]

References

Argay, Gy., Náray-Szabó, I., and Péter, É. (1969). J. Therm. Anal. 1, 413.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$ Internal standard W, $a = 3.16524 \text{ \AA}$ | | | |
|---|--------------------------------------|--------|-------------------|
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 3$ | hkl | $2\theta(^\circ)$ |
| 10.87 | 1L | 2 0 0 | 8.13 |
| 6.55 | 1L | 2 1 0 | 13.50 |
| 5.41M | 41 | 3 1 0 | 16.38 |
| 5.41M | | 4 0 0 | 16.38 |
| 5.32 | 21 | 0 1 1 | 16.66 |
| 5.03 | 5 | 1 1 1 | 17.61 |
| 4.591 | 15 | 2 1 1 | 19.32 |
| 4.526 | 10 | 4 1 0 | 19.60 |
| 4.075 | 5 | 3 1 1 | 21.79 |
| 4.032 | 7 | 1 2 0 | 22.03 |
| 4.005 | 2 | -4 1 1 | 22.18 |
| 3.831M | 9 | 2 2 0 | 23.20 |
| 3.831M | | 5 1 0 | 23.20 |
| 3.602M | 60 | 6 0 0 | 24.70 |
| 3.602M | | 4 1 1 | 24.70 |
| 3.530M | 20 | 0 2 1 | 25.21 |
| 3.530M | | -1 2 1 | 25.21 |
| 3.481 | 42 | 0 0 2 | 25.57 |
| 3.457 | 45 | -2 0 2 | 25.75 |
| 3.268M | 100 | 4 2 0 | 27.27 |
| 3.268M | | -3 2 1 | 27.27 |
| 3.186M | 44 | 2 0 2 | 27.98 |
| 3.186M | | -2 1 2 | 27.98 |
| 3.142 | 18 | -6 1 1 | 28.38 |
| 3.135 | 17 | -4 0 2 | 28.45 |
| 3.089M | 41 | 7 0 0 | 28.88 |
| 3.089M | | 3 2 1 | 28.88 |
| 2.978M | 5 | 5 2 0 | 29.98 |
| 2.978M | | 3 0 2 | 29.98 |
| 2.807 | 5 | -7 1 1 | 31.85 |
| 2.759 | 1 | 4 0 2 | 32.43 |
| 2.705 | 18 | 8 0 0 | 33.09 |
| 2.649M | 19 | 2 3 0 | 33.81 |
| 2.649M | | 5 2 1 | 33.81 |
| 2.567M | 4 | 8 1 0 | 34.92 |
| 2.567M | | -6 1 2 | 34.92 |
| 2.556M | 4 | 3 3 0 | 35.08 |
| 2.556M | | 7 1 1 | 35.08 |
| 2.522 | 2 | -8 1 1 | 35.57 |
| 2.432 | 3 | 5 1 2 | 36.93 |
| 2.411M | 1L | -7 2 1 | 37.26 |
| 2.411M | | 3 2 2 | 37.26 |
| 2.347 | 5 | 6 0 2 | 38.32 |
| 2.313M | 3 | 8 1 1 | 38.90 |
| 2.313M | | 5 3 0 | 38.90 |

Potassium Hydrogen Iodate, γ -KH(IO₃)₂ - (continued)

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 3$ | hkl | $2\theta(^{\circ})$ |
|-----------------|--------------------------------------|---------|---------------------|
| 2.283 | 1L | -9 1 1 | 39.43 |
| 2.250 | 4 | 7 2 1 | 40.04 |
| 2.163M | 2 | 10 0 0 | 41.72 |
| 2.163M | | 5 2 2 | 41.72 |
| 2.133M | 3 | -6 3 1 | 42.35 |
| 2.133M | | 2 1 3 | 42.35 |
| 2.107 | 2 | 9 1 1 | 42.89 |
| 2.092 | 3 | 10 1 0 | 43.22 |
| 2.075M | 6 | 2 3 2 | 43.59 |
| 2.075M | | 9 2 0 | 43.59 |
| 2.057M | 28 | -9 2 1 | 43.99 |
| 2.057M | | 3 1 3 | 43.99 |
| 2.054 | 25 | -9 1 2 | 44.05 |
| 2.034 | 24 | -1 2 3 | 44.51 |
| 2.004M | 9 | 8 0 2 | 45.22 |
| 2.004M | | -8 2 2 | 45.22 |
| 1.989 | 4 | 1 2 3 | 45.58 |
| 1.924+ | 7 | 8 3 0 | 47.20 |
| 1.924+ | | 2 4 1 | 47.20 |
| 1.912+ | 5 | -11 1 1 | 47.52 |
| 1.912+ | | -10 1 2 | 47.52 |
| 1.803 | 3 | 12 0 0 | 50.59 |
| 1.783+ | 9 | 11 1 1 | 51.19 |
| 1.783+ | | 6 4 0 | 51.19 |
| 1.768 | 7 | 0 4 2 | 51.67 |
| 1.763 | 6 | -3 3 3 | 51.83 |
| 1.750 | 9 | 5 2 3 | 52.23 |
| 1.729 | 8 | -4 0 4 | 52.91 |
| 1.725 | 7 | 2 4 2 | 53.06 |
| 1.717+ | 4 | 2 3 3 | 53.30 |
| 1.717+ | | -4 4 2 | 53.30 |
| 1.701 | 4 | -12 0 2 | 53.85 |
| 1.682 | 5 | 2 0 4 | 54.52 |
| 1.679M | 4 | 1 1 4 | 54.60 |
| 1.679M | | -5 4 2 | 54.60 |
| 1.669M | 5 | -10 1 3 | 54.96 |
| 1.669M | | 11 2 1 | 54.96 |
| 1.6484M | 4 | -9 2 3 | 55.72 |
| 1.6484M | | 2 1 4 | 55.72 |
| 1.6338M | 7 | 8 4 0 | 56.26 |
| 1.6338M | | -6 4 2 | 56.26 |
| 1.5962+ | 2 | 10 2 2 | 57.71 |
| 1.5962+ | | -10 3 2 | 57.71 |
| 1.5448+ | 1L | -4 5 1 | 59.82 |
| 1.5448+ | | 6 4 2 | 59.82 |

Potassium Hydrogen Oxalate Hydrate, $C_4H_3KO_8 \cdot 2H_2O$

Synonyms

1. Potassium trihydrogen oxalate dihydrate
2. Potassium tetroxalate

CAS registry no.

6100-20-5

Sample

NBS Standard Reference Material #189.

Color

Colorless

Structure

Triclinic, $P\bar{1}$ (2), $Z = 2$. The structure was determined by Haas (1964).

Lattice constants of this sample

$a = 7.031(2) \text{ \AA}$
 $b = 10.611(4)$
 $c = 6.367(2)$
 $\alpha = 101.36(3)^\circ$
 $\beta = 100.18(2)$
 $\gamma = 93.82(2)$

$a/b = 0.6626$

$c/b = 0.6000$

Volume

455.8 \AA^3

Density

(calculated) 1.852 g/cm^3

Figure of merit

$F_{30} = 40.6(0.017, 44)$

Reference intensity

$I/I_{\text{corundum}} = 1.14(7)$

Additional pattern

1. PDF card 14-845 [Dow Chemical Co., Midland, Michigan]

Reference

Haas, D. J. (1964). Acta Crystallogr. **17**, 1511.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$ | | | |
|---|--------------------------------------|--------|-------------------|
| Internal standard W, $a = 3.16524 \text{ \AA}$ | | | |
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 3$ | hkl | $2\theta(^\circ)$ |
| 6.13 | 9 | 0 0 1 | 14.43 |
| 6.04 | 8 | -1 1 0 | 14.66 |
| 5.85 | 1 | 0 -1 1 | 15.14 |
| 5.47 | 1 | 1 1 0 | 16.18 |
| 5.101 | 2 | -1 0 1 | 17.37 |

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 3$ | hkl | $2\theta(^\circ)$ |
|-----------------|--------------------------------------|---------|-------------------|
| 4.841 | 14 | 0 1 1 | 18.31 |
| 4.767 | 5 | -1 -1 1 | 18.60 |
| 4.451 | 13 | 0 -2 1 | 19.93 |
| 4.367 | 3 | -1 2 0 | 20.32 |
| 4.197 | 3 | 1 -1 1 | 21.15 |
| 3.943 | 3 | 1 2 0 | 22.53 |
| 3.828 | 2 | -1 -2 1 | 23.22 |
| 3.626 | 1 | 1 1 1 | 24.53 |
| 3.597 | 2 | 0 2 1 | 24.73 |
| 3.458 | 5 | -1 2 1 | 25.74 |
| 3.446 | 5 | 0 3 0 | 25.83 |
| 3.440 | 4 | 2 0 0 | 25.88 |
| 3.376 | 3 | -2 1 0 | 26.38 |
| 3.321 | 3 | 0 -3 1 | 26.82 |
| 3.283 | 4 | -2 0 1 | 27.14 |
| 3.143 | 100 | -2 -1 1 | 28.37 |
| 3.123 | 76 | 0 -1 2 | 28.56 |
| 3.064 | 28 | 0 0 2 | 29.12 |
| 3.041 | 7 | -1 -1 2 | 29.35 |
| 2.990 | 7 | 1 -3 1 | 29.86 |
| 2.963M | 7 | 1 2 1 | 30.14 |
| 2.963M | | 1 3 0 | 30.14 |
| 2.921 | 1 | 0 -2 2 | 30.58 |
| 2.820 | 8 | -1 -2 2 | 31.71 |
| 2.790 | 27 | -2 -2 1 | 32.05 |
| 2.783 | 22 | -1 1 2 | 32.14 |
| 2.757 | 9 | -2 2 1 | 32.45 |
| 2.658 | 7 | 2 -2 1 | 33.69 |
| 2.578M | 12 | 0 -3 2 | 34.77 |
| 2.578M | | 1 -2 2 | 34.77 |
| 2.544 | 4 | -2 0 2 | 35.25 |
| 2.531 | 7 | -2 -1 2 | 35.44 |
| 2.509 | 5 | -1 4 0 | 35.76 |
| 2.483 | 3 | -1 -3 2 | 36.15 |
| 2.442M | 20 | -1 2 2 | 36.78 |
| 2.442M | | 1 -4 1 | 36.78 |
| 2.426 | 6 | 1 3 1 | 37.03 |
| 2.412 | 6 | 1 1 2 | 37.25 |
| 2.394 | 4 | -2 -3 1 | 37.54 |
| 2.384 | 5 | 2 -3 1 | 37.70 |
| 2.361 | 13 | -2 3 1 | 38.08 |
| 2.348 | 8 | 1 -3 2 | 38.30 |
| 2.342 | 6 | 1 4 0 | 38.40 |
| 2.316 | 3 | 2 3 0 | 38.85 |
| 2.281 | 7 | 2 2 1 | 39.48 |
| 2.257 | 2 | -3 1 1 | 39.91 |
| 2.232 | 6 | -3 -1 1 | 40.37 |
| 2.199 | 3 | -2 2 2 | 41.01 |
| 2.184 | 5 | -3 2 0 | 41.30 |
| 2.146 | 7 | -1 -4 2 | 42.07 |

Potassium Hydrogen Oxalate Hydrate, $C_4H_3KO_8 \cdot 2H_2O$ - (continued)

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 3$ | hkl | $2\theta(^{\circ})$ |
|-----------------|-------------------------------|---------|---------------------|
| 2.100M | 2 | 2 -2 2 | 43.04 |
| 2.100M | | 0 -5 1 | 43.04 |
| 2.094 | 3 | 2 0 2 | 43.17 |
| 2.083 | 2 | -3 -2 1 | 43.41 |
| 2.068M | 4 | -1 0 3 | 43.73 |
| 2.068M | | 0 5 0 | 43.73 |
| 2.053 | 5 | 0 -2 3 | 44.07 |
| 2.049 | 3 | 3 -1 1 | 44.16 |
| 2.040M | 3 | 0 0 3 | 44.36 |
| 2.040M | | -1 5 0 | 44.36 |
| 2.015 | 2 | -3 -1 2 | 44.94 |
| 2.009 | 2 | -3 3 0 | 45.09 |
| 1.998 | 7 | 3 -2 1 | 45.35 |

Potassium Niobium Oxide, KNbO_3

Synonym

1. Potassium niobate

CAS registry no.

12030-85-2

Sample

The sample was a Johnson Matthey chemical obtained from Ventron Corp., Danvers, MA.

Major impurities

The manufacturer's spectrographic analysis showed ≈ 3 ppm silicon.

Color

Colorless

Structure

Orthorhombic, $\text{Cm}2\text{m}$ (38), $Z = 2$, iso-structural with the distorted perovskite form of BaTiO_3 . The structure was determined by Katz and Megaw [1954].

Lattice constants of this sample

$a = 5.6950(4) \text{ \AA}$
 $b = 5.7213(3)$
 $c = 3.9739(2)$

$a/b = 0.9954$
 $c/b = 0.6946$

Volume

129.48 \AA^3

Density

(calculated) 4.167 g/cm^3

Figure of merit

$F_{30} = 96.0(0.009,35)$

Reference intensity

$I/I_{\text{corundum}} = 5.26(12)$

Polymorphism

Potassium niobium oxide crystallizes in three modifications, orthorhombic at room temperature, changing to tetragonal at about 255°C and cubic near 435°C [Wood, 1951].

Additional pattern

1. PDF card 9-156 [Wood, priv. comm.]

References

Katz, L. and Megaw, H. D. (1967). Acta Crystallogr. **22**, 639.
 Wood, E. A. (1951). Acta Crystallogr. **4**, 353.

| CuK α_1 $\lambda = 1.540598$ Å; temp. 25 ± 1 °C | | | | | |
|--|------------------|-------|---|---|---------------------|
| Internal standard W, $a = 3.16524$ Å | | | | | |
| $d(\text{Å})$ | I^{rel} | hkl | | | $2\theta(^{\circ})$ |
| $\sigma = \pm 1$ | | | | | |
| 4.035 | 47 | 1 | 1 | 0 | 22.01 |
| 3.973 | 22 | 0 | 0 | 1 | 22.36 |
| 2.859 | 36 | 0 | 2 | 0 | 31.26 |
| 2.848 | 46 | 2 | 0 | 0 | 31.39 |
| 2.832 | 100 | 1 | 1 | 1 | 31.57 |
| 2.322 | 1 | 0 | 2 | 1 | 38.75 |
| 2.0180 | 33 | 2 | 2 | 0 | 44.88 |
| 1.9866 | 16 | 0 | 0 | 2 | 45.63 |
| 1.8081 | 3 | 1 | 3 | 0 | 50.43 |
| 1.7998 | 9 | 2 | 2 | 1 | 50.68 |
| 1.7831 | 6 | 1 | 1 | 2 | 51.19 |
| 1.6462 | 15 | 1 | 3 | 1 | 55.80 |
| 1.6413 | 19 | 3 | 1 | 1 | 55.98 |
| 1.6314 | 11 | 0 | 2 | 2 | 56.35 |
| 1.6296 | 6 | 2 | 0 | 2 | 56.42 |
| 1.4305 | 2 | 0 | 4 | 0 | 65.16 |
| 1.4239 | 4 | 4 | 0 | 0 | 65.50 |
| 1.4160 | 13 | 2 | 2 | 2 | 65.91 |
| 1.3458M | 1 | 0 | 4 | 1 | 69.83 |
| 1.3458M | | 3 | 3 | 0 | 69.83 |
| 1.3405 | 1 | 4 | 0 | 1 | 70.15 |
| 1.3371 | 2 | 1 | 3 | 2 | 70.35 |
| 1.3347 | 2 | 3 | 1 | 2 | 70.50 |
| 1.3249 | 1L | 0 | 0 | 3 | 71.10 |
| 1.2782 | 2 | 2 | 4 | 0 | 74.12 |
| 1.2746M | 7 | 4 | 2 | 0 | 74.36 |
| 1.2746M | | 3 | 3 | 1 | 74.36 |
| 1.2586 | 4 | 1 | 1 | 3 | 75.47 |
| 1.2169 | 1L | 2 | 4 | 1 | 78.54 |
| 1.2137 | 1L | 4 | 2 | 1 | 78.79 |
| 1.2020 | 1L | 0 | 2 | 3 | 79.71 |
| 1.1610 | 2 | 0 | 4 | 2 | 83.13 |
| 1.1576 | 3 | 4 | 0 | 2 | 83.43 |
| 1.1221 | 1L | 1 | 5 | 0 | 86.70 |
| 1.1170 | 1L | 5 | 1 | 0 | 87.20 |
| 1.1142 | 1L | 3 | 3 | 2 | 87.47 |
| 1.1075 | 1L | 2 | 2 | 3 | 88.14 |
| 1.0797 | 1 | 1 | 5 | 1 | 91.03 |
| 1.0751M | 3 | 5 | 1 | 1 | 91.53 |
| 1.0751M | | 2 | 4 | 2 | 91.53 |
| 1.0727 | 3 | 4 | 2 | 2 | 91.79 |
| 1.0687 | 3 | 1 | 3 | 3 | 92.24 |
| 1.0674 | 2 | 3 | 1 | 3 | 92.38 |
| 1.0091 | 1 | 4 | 4 | 0 | 99.52 |
| .9934 | 1L | 0 | 0 | 4 | 101.68 |

Potassium Niobium Oxide, KNbO_3 - (continued)

| d(Å) | I ^{rel} | hkl | | | 2θ(°) |
|--------|------------------|-----|---|---|--------|
| σ = ±1 | | | | | |
| .9801 | 1L | 3 | 5 | 0 | 103.62 |
| .9780M | 1L | 4 | 4 | 1 | 103.93 |
| .9780M | | 5 | 3 | 0 | 103.93 |
| .9769 | 1L | 1 | 5 | 2 | 104.10 |
| .9738 | 1L | 5 | 1 | 2 | 104.57 |
| | | | | | |
| .9696 | 1L | 4 | 0 | 3 | 105.20 |
| .9646 | 1L | 1 | 1 | 4 | 105.99 |
| .9534 | 1L | 0 | 6 | 0 | 107.79 |
| .9514 | 1 | 3 | 5 | 1 | 108.13 |
| .9494M | 2 | 5 | 3 | 1 | 108.46 |
| .9494M | | 6 | 0 | 0 | 108.46 |
| .9438 | 1 | 3 | 3 | 3 | 109.41 |
| .9381 | 1 | 2 | 0 | 4 | 110.40 |
| .9272 | 1L | 0 | 6 | 1 | 112.35 |
| .9231 | 1L | 6 | 0 | 1 | 113.12 |
| | | | | | |
| .9197 | 1L | 2 | 4 | 3 | 113.76 |

Potassium Sulfate, $K_2S_2O_8$

Synonym

1. Potassium persulfate

CAS registry no.

7727-21-1

Sample

The sample was obtained from the Fisher Scientific Co., Fair Lawn, NJ. and was recrystallized from an aqueous solution.

Color

Colorless

Structure

Triclinic, $Z = 1$ (assuming a density near 2.5). The cell was obtained by V. Himes using a single crystal on a diffractometer. The cell was confirmed by the Visser program [1969]. Two somewhat different triclinic cells were reported in the literature [Keen, 1935 and Gerstäcker et al., 1928]. Our data did not index on either of these cells.

Lattice constants of this sample

$a = 5.514(2) \text{ \AA}$
 $b = 7.038(2)$
 $c = 5.116(2)$
 $\alpha = 106.11(2)^\circ$
 $\beta = 90.15(3)$
 $\gamma = 106.30(3)$

$a/b = 0.7835$
 $c/b = 0.7269$

Volume

182.38 \AA^3

Density

(calculated) 2.461 g/cm^3
(measured) 2.45 g/cm^3

Figures of merit

$F_{30} = 34.9(0.016, 52)$
 $M_{20} = 27.3$

Reference intensity

$I/I_{\text{corundum}} = 1.31(7)$

Additional pattern

1. PDF card 12-483 [Institute of Physics, University College, Cardiff, Wales].

References

Gerstäcker, A., Möller, H., and Reis, A. (1928). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 66, 421.
Keen, R. C. (1935). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 91, 129.
Visser, J. W. (1969). J. Appl. Crystallogr.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$ | | | | |
|---|--------------------------------------|---------|-------------------|--|
| Internal standard Si, $a = 5.43088 \text{ \AA}$ | | | | |
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 4$ | hkl | $2\theta(^\circ)$ | |
| 5.27 | 2 | 1 0 0 | 16.80 | |
| 4.892 | 15 | 0 0 1 | 18.12 | |
| 4.847 | 20 | -1 1 0 | 18.29 | |
| 4.602 | 1L | 0 -1 1 | 19.27 | |
| 3.750 | 9 | -1 0 1 | 23.71 | |
| 3.699 | 38 | 1 -1 1 | 24.04 | |
| 3.603 | 4 | 1 1 0 | 24.69 | |
| 3.443 | 52 | 1 0 1 | 25.86 | |
| 3.268 | 56 | -1 -1 1 | 27.27 | |
| 3.232M | 100 | 0 2 0 | 27.58 | |
| 3.232M | | -1 1 1 | 27.58 | |
| 3.153 | 3 | 0 -2 1 | 28.28 | |
| 3.025 | 11 | 1 -2 1 | 29.50 | |
| 2.736 | 14 | -2 1 0 | 32.71 | |
| 2.634M | 9 | 1 1 1 | 34.01 | |
| 2.634M | | 2 0 0 | 34.01 | |
| 2.548 | 10 | 0 -1 2 | 35.20 | |
| 2.466 | 22 | -1 -2 1 | 36.40 | |
| 2.419 | 10 | -2 2 0 | 37.13 | |
| 2.397 | 5 | 0 2 1 | 37.49 | |
| 2.358 | 3 | -2 1 1 | 38.14 | |
| 2.315 | 3 | 1 -1 2 | 38.87 | |
| 2.297+ | 5 | -1 0 2 | 39.18 | |
| 2.297+ | | 2 -2 1 | 39.18 | |
| 2.273M | 3 | 1 -3 1 | 39.62 | |
| 2.273M | | -1 -1 2 | 39.62 | |
| 2.239M | 2 | 2 0 1 | 40.25 | |
| 2.239M | | -1 3 0 | 40.25 | |
| 2.224M | 1 | 0 -3 1 | 40.52 | |
| 2.224M | | 2 1 0 | 40.52 | |
| 2.154 | 3 | 0 3 0 | 41.90 | |
| 2.098 | 1 | 0 1 2 | 43.08 | |
| 1.995 | 5 | 1 2 1 | 45.42 | |
| 1.975M | 7 | -2 3 0 | 45.91 | |
| 1.975M | | 2 -3 1 | 45.91 | |
| 1.923 | 10 | 1 -3 2 | 47.22 | |
| 1.917 | 4 | 0 -3 2 | 47.39 | |
| 1.881 | 7 | -1 -3 1 | 48.35 | |
| 1.858 | 2 | -1 3 1 | 48.98 | |
| 1.853 | 2 | 2 -2 2 | 49.14 | |
| 1.844 | 1 | 1 1 2 | 49.39 | |
| 1.809 | 5 | -2 -1 2 | 50.40 | |
| 1.800 | 7 | 2 2 0 | 50.66 | |
| 1.753 | 2 | 1 -4 1 | 52.14 | |
| 1.711 | 3 | 3 -2 1 | 53.51 | |

Potassium Sulfate, $K_2S_2O_8$ - (continued)

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 4$ | hkl | $2\theta(^{\circ})$ |
|-----------------|--------------------------------------|---------|---------------------|
| 1.6338M | 3 | -3 2 1 | 56.26 |
| 1.6338M | | -2 -2 2 | 56.26 |
| 1.6154M | 8 | 1 -2 3 | 56.96 |
| 1.6154M | | 1 -1 3 | 56.96 |
| 1.6138M | 4 | 1 -4 2 | 57.02 |
| 1.6138M | | -2 2 2 | 57.02 |

Scandium Boride, ScB₂

CAS registry no.
12007-34-0

Sample

The sample was obtained from Cerac, Menomonee Falls, WI.

Color

Metallic gray

Structure

Hexagonal, P6/mmm (191) Z = 1. The structure was qualitatively done by Zhuravlev and Stepanova [1958].

Lattice constants of this sample

a = 3.14573(12) Å
c = 3.5175(2)

c/a = 1.1182

Volume

30.145 Å³

Density

(calculated) 3.667 g/cm³

Figure of merit

F₁₉ = 73.3(0.011,23)

Additional pattern

1. PDF card 11-527 [Zhuravlev and Stepanova, 1958].

References

Zhuravlev, N. N. and Stepanova, A. A. (1958). Kristallografiya 3, 83.

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C Internal standard W, a = 3.16524 Å | | | | |
|---|----------------------------|-------|--------|--|
| d(Å) | I ^{rel} σ = ±2 | hkl | 2θ(°) | |
| 3.517 | 17 | 0 0 1 | 25.30 | |
| 2.725 | 51 | 1 0 0 | 32.84 | |
| 2.153 | 100 | 1 0 1 | 41.92 | |
| 1.7594 | 10 | 0 0 2 | 51.93 | |
| 1.5733 | 18 | 1 1 0 | 58.63 | |
| 1.4774 | 13 | 1 0 2 | 62.85 | |
| 1.4358 | 8 | 1 1 1 | 64.89 | |
| 1.3619 | 5 | 2 0 0 | 68.89 | |
| 1.2703 | 12 | 2 0 1 | 74.66 | |
| 1.1721M | 12 | 0 0 3 | 82.17 | |
| 1.1721M | | 1 1 2 | 82.17 | |
| 1.0768M | 8 | 1 0 3 | 91.34 | |
| 1.0768M | | 2 0 2 | 91.34 | |
| 1.0297 | 3 | 2 1 0 | 96.85 | |
| .9883 | 8 | 2 1 1 | 102.42 | |
| .9401 | 1L | 1 1 3 | 110.05 | |
| .9081 | 3 | 3 0 0 | 116.05 | |
| .8885M | 6 | 2 0 3 | 120.21 | |
| .8885M | | 2 1 2 | 120.21 | |
| .8792M | 2 | 0 0 4 | 122.35 | |
| .8792M | | 3 0 1 | 122.35 | |
| .8369 | 2 | 1 0 4 | 133.99 | |
| .8069 | 3 | 3 0 2 | 145.36 | |

Silver Mercury Iodide, β -Ag₂HgI₄

CAS registry no.
7784-03-4

Sample

The sample was obtained from Ventron Corp.
(Alfa), Danvers, MA.

Color

Vivid yellow

Structure

Tetragonal, $I\bar{4}$ (82), $Z = 2$, pseudocubic.
The structure of β -Ag₂HgI₄ was determined by
Hahn et al. [1955]. A cell with $c/2$ was
reported by Ketelaar [1931] and a cell with
2a was reported by Frevel and North [1950].

Lattice constants of this sample

$a = 6.3302(8) \text{ \AA}$
 $c = 12.624(2)$

$c/a = 1.9942$

Volume
 505.88 \AA^3

Density

(calculated) 6.069 g/cm^3

Figure of merit

$F_{30} = 47.1(0.016, 41)$

Reference intensity

$I/I_{\text{corundum}} = 5.60(10)$

Polymorphism

Above 60°C , Ag₂HgI₄ is cubic [Ketelaar,
1931]. Otsubo [1966] reports another
form of Ag₂HgI₄ as hexagonal and stable
above 165°C .

Additional patterns

1. PDF card 3-0949 [Ketelaar, 1931]
2. PDF card 4-0442 [Frevel and North,
1950]
3. PDF card 18-1183 [Hahn et al., 1955]

References

- Frevel, L. K. and North, P. P. (1950). J.
Appl. Phys. **21**, 1038.
Hahn, H., Frank, G., and Klingler, W. (1955).
Z. Anorg. Allgem. Chem. **279**, 271.
Ketelaar, J. A. A. (1931). Z. Kristallogr.
Kristallgeometrie Kristallphys.
Kristallchem. **80**, 192.
Otsubo, Y., Nitta, A., Kaneko, M., Iwata, Y.,
and Ueki, A. (1966). Kogyo Kagaku
Zasshi **69**, 1716.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ\text{C}$ Internal standard Si, $a = 5.43088 \text{ \AA}$ | | | |
|---|--------------------------------------|-------|-------------------|
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 1$ | hkl | $2\theta(^\circ)$ |
| 6.30 | 3 | 0 0 2 | 14.05 |
| 5.64 | 6 | 1 0 1 | 15.69 |
| 4.471 | 6 | 1 1 0 | 19.84 |
| 3.650 | 100 | 1 1 2 | 24.37 |
| 3.502 | 5 | 1 0 3 | 25.41 |
| 3.163 | 1L | 2 0 0 | 28.19 |
| 3.156 | 1L | 0 0 4 | 28.25 |
| 2.828 | 5 | 2 0 2 | 31.61 |
| 2.761 | 5 | 2 1 1 | 32.40 |
| 2.578 | 4 | 1 1 4 | 34.77 |
| 2.347M | 3 | 2 1 3 | 38.32 |
| 2.347M | | 1 0 5 | 38.32 |
| 2.236 | 45 | 2 0 4 | 40.31 |
| 2.103 | 2 | 0 0 6 | 42.97 |
| 2.081 | 2 | 3 0 1 | 43.46 |
| 2.002 | 1 | 3 1 0 | 45.27 |
| 1.908 | 19 | 3 1 2 | 47.62 |
| 1.904 | 18 | 1 1 6 | 47.72 |
| 1.884 | 1 | 2 1 5 | 48.26 |
| 1.7385 | 1L | 3 2 1 | 52.60 |
| 1.7340 | 1L | 1 0 7 | 52.75 |
| 1.6907 | 1L | 3 1 4 | 54.21 |
| 1.6203 | 1 | 3 2 3 | 56.77 |
| 1.5829 | 3 | 4 0 0 | 58.24 |
| 1.5782 | 3 | 0 0 8 | 58.43 |
| 1.5332 | 1 | 2 2 6 | 60.32 |
| 1.5240 | 1L | 4 1 1 | 60.72 |
| 1.5206 | 1L | 2 1 7 | 60.87 |
| 1.4887 | 1L | 1 1 8 | 62.32 |
| 1.4508 | 4 | 3 1 6 | 64.14 |
| 1.4416M | 2 | 4 1 3 | 64.60 |
| 1.4416M | | 3 2 5 | 64.60 |
| 1.3813 | 1L | 4 2 2 | 67.79 |
| 1.3494 | 1L | 3 3 4 | 69.62 |
| 1.3119 | 1L | 4 1 5 | 71.91 |
| 1.2917 | 4 | 4 2 4 | 73.22 |
| 1.2901 | 3 | 2 2 8 | 73.32 |
| 1.2643 | 1L | 4 0 6 | 75.07 |

Sodium Chlorate Hydrate, $\text{NaClO}_4 \cdot \text{H}_2\text{O}$

Synonym

1. Sodium perchlorate hydrate

CAS registry no.

7791-07-3

Sample

The sample was recrystallized from reagent material received from the Fisher Scientific Co., Fair Lawn, NJ. The crystals were very unstable, changing readily to the anhydrous phase and back again depending on the atmospheric relative humidity.

* Because of the sample's instability, the intensities were calculated from the structure data given by Berglund et al. [1975].

Color

Colorless

Structure

Monoclinic, C2/c (15), $Z = 8$. The structure was refined by Berglund et al. [1975].

Lattice constants of this sample

$a = 15.555(3) \text{ \AA}$
 $b = 5.5436(9)$
 $c = 11.063(3)$
 $\beta = 110.70(2)^\circ$

 $a/b = 2.8059$ $c/b = 1.9956$

Volume

 892.4 \AA^3

Density

(calculated) 2.091 g/cm^3

Figure of merit

 $F_{30} = 26.0 (0.015, 78)$

Reference intensity

$I/I_{\text{corundum}} = 1.34$ (calculated from the structural data)

Additional pattern

1. PDF card 28-1071 [Hanawalt et al., 1938]

References

Berglund, B., Thomas, J. O., and Tellgren, R. (1975). *Acta Crystallogr.* B31, 1842.
 Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). *Ind. Eng. Chem. Anal. Ed.* 10, 457.

 $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$ Internal standard W, $a = 3.16524 \text{ \AA}$

| $d(\text{\AA})$ | I^* | hkl | $2\theta(^\circ)$ |
|-----------------|-------|--------|-------------------|
| 5.18M | 44 | 1 1 0 | 17.10 |
| 5.18M | | 0 0 2 | 17.10 |
| 4.894 | 2 | -1 1 1 | 18.11 |
| 4.421 | 6 | 1 1 1 | 20.07 |
| 3.648+ | 77 | 2 0 2 | 24.38 |
| 3.648+ | | 3 1 0 | 24.38 |
| 3.445M | 100 | 1 1 2 | 25.84 |
| 3.445M | | -3 1 2 | 25.84 |
| 3.187 | 5 | 3 1 1 | 27.97 |
| 2.928 | 3 | -3 1 3 | 30.51 |
| 2.771 | 9 | 0 2 0 | 32.28 |
| 2.764 | 11 | -2 0 4 | 32.36 |
| 2.707 | 3 | -5 1 1 | 33.06 |
| 2.666 | 4 | 3 1 2 | 33.59 |
| 2.660 | 3 | -5 1 2 | 33.66 |
| 2.592M | 1 | -2 2 1 | 34.58 |
| 2.592M | | 2 2 0 | 34.58 |
| 2.585M | 1L | 0 0 4 | 34.67 |
| 2.585M | | -4 0 4 | 34.67 |
| 2.577M | 1L | 4 0 2 | 34.78 |
| 2.577M | | 5 1 0 | 34.78 |
| 2.467 | 1 | -5 1 3 | 36.39 |
| 2.443+ | 5 | 0 2 2 | 36.76 |
| 2.443+ | | -2 2 2 | 36.76 |
| 2.437 | 5 | -3 1 4 | 36.86 |
| 2.228 | 1 | 3 1 3 | 40.45 |
| 2.205+ | 16 | 4 2 0 | 40.90 |
| 2.205+ | | 2 0 4 | 40.90 |
| 2.162 | 1 | 0 2 3 | 41.75 |
| 2.063 | 4 | 5 1 2 | 43.85 |
| 2.060 | 3 | -7 1 2 | 43.92 |
| 2.040 | 1 | -7 1 1 | 44.36 |
| 2.011 | 1 | -1 1 5 | 45.04 |
| 1.958M | 1 | -2 2 4 | 46.33 |
| 1.958M | | 2 2 3 | 46.33 |
| 1.947M | 1 | 6 0 2 | 46.61 |
| 1.947M | | 7 1 0 | 46.61 |
| 1.885M | 2 | -6 2 2 | 48.23 |
| 1.885M | | -6 2 1 | 48.23 |
| 1.844 | 1L | 1 1 5 | 49.39 |
| 1.825M | 7 | 4 0 4 | 49.93 |
| 1.825M | | 6 2 0 | 49.93 |
| 1.820M | 8 | -8 0 4 | 50.07 |
| 1.820M | | -1 3 1 | 50.07 |
| 1.811 | 1L | 5 1 3 | 50.35 |
| 1.792 | 1L | 1 3 1 | 50.92 |
| 1.739 | 2 | -3 3 1 | 52.57 |
| 1.724M | 9 | 0 0 6 | 53.08 |
| 1.724M | | -6 2 4 | 53.08 |
| 1.722M | 8 | -6 0 6 | 53.16 |

Sodium Chlorate Hydrate $\text{NaClO}_4 \cdot \text{H}_2\text{O}$ - (continued)

| $d(\text{\AA})$ | I^* | hkl | $2\theta(^{\circ})$ |
|-----------------|-------|---------|---------------------|
| 1.722M | | 6 2 1 | 53.16 |
| 1.7040M | 1 | 1 3 2 | 53.75 |
| 1.7040M | | -3 3 2 | 53.75 |
| 1.7017M | 3 | -1 1 6 | 53.83 |
| 1.7017M | | -4 2 5 | 53.83 |
| 1.6691 | 1 | 3 3 1 | 54.97 |
| 1.6497M | 1L | 7 1 2 | 55.67 |
| 1.6497M | | -1 3 3 | 55.67 |
| 1.5919 | 1 | -8 2 2 | 57.88 |
| 1.5794M | 1 | 3 3 2 | 58.38 |
| 1.5794M | | -5 3 2 | 58.38 |
| 1.5514M | 1L | 9 1 0 | 59.54 |
| 1.5514M | | -10 0 2 | 59.54 |
| 1.5254M | 1 | 2 2 5 | 60.66 |
| 1.5254M | | 4 2 4 | 60.66 |
| 1.5202 | 2 | 8 2 0 | 60.89 |
| 1.5126 | 1L | -9 1 5 | 61.23 |
| 1.5006M | 1L | 5 3 1 | 61.77 |
| 1.5006M | | -5 1 7 | 61.77 |
| 1.4199M | 2 | 3 1 6 | 65.71 |
| 1.4199M | | -7 3 2 | 65.71 |
| 1.4162 | 3 | -3 3 5 | 65.90 |
| 1.3860 | 1 | 0 4 0 | 67.53 |
| 1.3816M | 2 | 7 3 0 | 67.77 |
| 1.3816M | | 4 0 6 | 67.77 |
| 1.3734 | 1 | 0 4 1 | 68.23 |
| 1.3631 | 1 | -11 1 2 | 68.82 |
| 1.3543+ | 1 | 7 1 4 | 69.33 |
| 1.3543+ | | 8 2 2 | 69.33 |
| 1.3385+ | 1L | -2 4 2 | 70.27 |
| 1.3385+ | | 2 4 1 | 70.27 |
| 1.3342M | 1 | -11 1 1 | 70.53 |
| 1.3342M | | 6 2 4 | 70.53 |
| 1.3309M | 1 | -10 2 4 | 70.73 |
| 1.3309M | | -10 2 1 | 70.73 |
| 1.2953M | 1 | -4 4 2 | 72.98 |
| 1.2953M | | 4 4 0 | 72.98 |

Sodium L(+)-Glutamate Hydrate, $C_5H_8NNaO_4 \cdot H_2O$

Synonym

1. Monosodium glutamate hydrate
2. Accent

CAS registry no.

142-47-2

Sample

The sample was manufactured by the Ajinomoto Co., Japan, and purchased as a food additive. It was recrystallized from a mixture of water and ethanol.

Color

Colorless

Structure

Orthorhombic, $P2_12_12_1(19)$, $Z = 8$. The unit cell and space group were determined by Uno [1952].

Lattice constants of this sample

 $a = 15.235(3) \text{ \AA}$ $b = 17.937(4)$ $c = 5.667(2)$ $a/b = 0.8494$ $c/b = 0.3104$

Volume

 1521.3 \AA^3

Density

(calculated) 1.634 g/cm^3

Figure of merit

 $F_{30} = 45.6(0.014, 48)$

Reference intensity

 $I/I_{\text{corundum}} = 0.35(2)$

Additional pattern

1. PDF card 18-1904 [Institute of Physics, University College, Cardiff, Wales]

Reference

Uno, T., (1952). Yokugaku Zasshi (J. Pharm. Soc. Japan) 72, 26.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$ Internal standard Si, $a = 5.43088 \text{ \AA}$ | | | |
|--|--------------------------------------|-------|-------------------|
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 2$ | hkl | $2\theta(^\circ)$ |
| 11.62 | 3 | 1 1 0 | 7.60 |
| 8.95 | 10 | 0 2 0 | 9.87 |
| 7.72 | 10 | 1 2 0 | 11.46 |
| 7.61 | 4 | 2 0 0 | 11.62 |
| 7.02 | 3 | 2 1 0 | 12.60 |
| 5.80 | 15 | 2 2 0 | 15.27 |
| 5.562 | 5 | 1 3 0 | 15.92 |
| 5.024 | 8 | 1 1 1 | 17.64 |
| 4.886 | 2 | 3 1 0 | 18.14 |
| 4.697 | 4 | 2 3 0 | 18.88 |
| 4.519 | 95 | 1 2 1 | 19.63 |
| 4.416 | 75 | 3 2 0 | 20.09 |
| 4.358 | 39 | 2 1 1 | 20.36 |
| 4.298 | 6 | 1 4 0 | 20.65 |
| 4.017 | 38 | 2 2 1 | 22.11 |
| 3.935 | 24 | 1 3 1 | 22.58 |
| 3.860 | 32 | 2 4 0 | 23.02 |
| 3.807 | 88 | 4 0 0 | 23.35 |
| 3.728 | 33 | 4 1 0 | 23.85 |
| 3.589 | 33 | 2 3 1 | 24.79 |
| 3.505 | 100 | 4 2 0 | 25.39 |
| 3.460 | 17 | 3 2 1 | 25.73 |
| 3.402 | 18 | 1 4 1 | 26.17 |
| 3.361 | 12 | 3 4 0 | 26.50 |
| 3.209 | 24 | 4 3 0 | 27.78 |
| 3.175M | 74 | 3 3 1 | 28.08 |
| 3.175M | | 2 4 1 | 28.08 |
| 3.141 | 19 | 4 0 1 | 28.39 |
| 3.096 | 19 | 4 1 1 | 28.81 |
| 2.958 | 16 | 1 5 1 | 30.19 |
| 2.931M | 8 | 1 6 0 | 30.47 |
| 2.931M | | 3 5 0 | 30.47 |
| 2.901 | 19 | 4 4 0 | 30.80 |
| 2.879 | 37 | 3 4 1 | 31.04 |
| 2.802 | 16 | 2 5 1 | 31.91 |
| 2.784+ | 8 | 0 0 2 | 32.12 |
| 2.784+ | | 2 6 0 | 32.12 |
| 2.715 | 2 | 5 3 0 | 32.97 |
| 2.706 | 2 | 1 1 2 | 33.08 |
| 2.642 | 9 | 5 1 1 | 33.90 |
| 2.633 | 14 | 0 6 1 | 34.02 |
| 2.612M | 25 | 2 0 2 | 34.30 |
| 2.612M | | 4 5 0 | 34.30 |
| 2.593M | 29 | 1 6 1 | 34.57 |
| 2.593M | | 3 5 1 | 34.57 |

Sodium L(+)-Glutamate Hydrate, $C_5H_8NNaO_4 \cdot H_2O$ - (continued)

| $d(A)$ | I^{rel} $\sigma = \pm 2$ | hkl | $2\theta(^{\circ})$ |
|--------|-------------------------------|-------|---------------------|
| 2.562 | 7 | 5 2 1 | 35.00 |
| 2.525M | 9 | 1 7 0 | 35.53 |
| 2.525M | | 0 3 2 | 35.53 |
| 2.521 | 9 | 5 4 0 | 35.58 |
| 2.489M | 26 | 1 3 2 | 36.06 |
| 2.489M | | 2 6 1 | 36.06 |
| 2.441+ | 16 | 6 2 0 | 36.79 |
| 2.441+ | | 3 0 2 | 36.79 |
| 2.362 | 11 | 4 5 1 | 38.06 |
| 2.356 | 12 | 3 2 2 | 38.16 |
| 2.352 | 17 | 4 6 0 | 38.24 |
| 2.338+ | 9 | 3 6 1 | 38.48 |
| 2.338+ | | 6 3 0 | 38.48 |
| 2.310 | 8 | 6 0 1 | 38.96 |
| 2.301 | 16 | 1 7 1 | 39.11 |
| 2.296 | 17 | 5 4 1 | 39.21 |
| 2.258M | 16 | 3 3 2 | 39.90 |
| 2.258M | | 2 4 2 | 39.90 |
| 2.237 | 24 | 6 2 1 | 40.28 |
| 2.230 | 22 | 4 1 2 | 40.42 |
| 2.227 | 19 | 2 7 1 | 40.48 |
| 2.200 | 12 | 0 5 2 | 41.00 |
| 2.167 | 41 | 4 6 1 | 41.65 |
| 2.144M | 6 | 3 4 2 | 42.12 |
| 2.144M | | 5 5 1 | 42.12 |
| 2.135 | 4 | 5 6 0 | 42.29 |
| 2.126 | 4 | 4 7 0 | 42.49 |
| 2.115M | 6 | 3 7 1 | 42.71 |
| 2.115M | | 7 2 0 | 42.71 |
| 2.060 | 5 | 1 8 1 | 43.92 |
| 2.052 | 9 | 3 8 0 | 44.10 |
| 2.037 | 4 | 0 6 2 | 44.44 |
| 1.994 | 7 | 5 6 1 | 45.46 |
| 1.987 | 5 | 4 7 1 | 45.62 |
| 1.959 | 7 | 7 4 0 | 46.31 |

Sodium Hydrogen Oxalate Hydrate, $C_2HNaO_4 \cdot H_2O$

Synonym

1. Sodium binoxalate hydrate
2. Sodium acid oxalate hydrate

CAS registry no.

16009-94-2

Sample

The sample was obtained from Fisher Scientific Co., Fair Lawn, N. J. It was recrystallized from a hot aqueous solution to which a small amount of $H_2C_2O_4$ was added. The sample was mounted in Canada Balsam for the intensity measurements. Since the material exhibited strong cleavage and a tendency to lose H_2O , the intensity determinations may be subject to some error.

Color

Colorless

Structure

Triclinic, $P\bar{1}$ (2), $Z = 2$ [Hendricks, 1935].

Lattice constants of this sample

$a = 6.516(2) \text{ \AA}$
 $b = 6.675(2)$
 $c = 5.708(2)$
 $\alpha = 95.06(4)^\circ$
 $\beta = 109.96(4)$
 $\gamma = 75.03(2)$

 $a/b = 0.9762$ $c/b = 0.8551$

Volume

 225.43 \AA^3

Density

(calculated) 1.916 g/cm^3

Figure of merit

 $F_{30} = 26.2(0.016, 71)$

Additional pattern

1. PDF card 14-755 [Hanawalt et al., 1938]

References

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K.
 (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
 Hendricks, S. B. (1935). Z. Kristallogr.
 Kristallgeometrie Kristallphys. Kristallchem.
92, 301.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$ Internal standard W, $a = 3.16524 \text{ \AA}$ | | | |
|---|--------------------------------------|---------|-------------------|
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 3$ | hkl | $2\theta(^\circ)$ |
| 6.44 | 4 | 0 1 0 | 13.73 |
| 5.93 | 1L | 1 0 0 | 14.92 |
| 5.36 | 14 | 0 0 1 | 16.53 |
| 5.027 | 3 | 1 1 0 | 17.63 |
| 4.862 | 14 | -1 0 1 | 18.23 |
| 4.318 | 11 | -1 -1 1 | 20.55 |
| 4.132M | 10 | 0 -1 1 | 21.49 |
| 4.132M | | 0 1 1 | 21.49 |
| 3.919 | 10 | -1 1 0 | 22.67 |
| 3.226 | 14 | 0 2 0 | 27.63 |
| 3.179 | 12 | 1 2 0 | 28.05 |
| 3.084 | 4 | -2 -1 1 | 28.93 |
| 2.987 | 32 | 2 1 0 | 29.89 |
| 2.968 | 100 | 2 0 0 | 30.08 |
| 2.683 | 21 | 0 0 2 | 33.37 |
| 2.583 | 6 | -1 2 0 | 34.70 |
| 2.568 | 1L | -2 -2 1 | 34.91 |
| 2.530 | 7 | -2 1 1 | 35.45 |
| 2.482 | 24 | -1 1 2 | 36.16 |
| 2.477+ | 18 | 0 -1 2 | 36.24 |
| 2.477+ | | 0 1 2 | 36.24 |
| 2.442 | 8 | -2 -1 2 | 36.77 |
| 2.306 | 3 | 2 1 1 | 39.03 |
| 2.256 | 5 | -1 -2 2 | 39.93 |
| 2.165 | 8 | -3 -1 1 | 41.69 |
| 2.131M | 9 | 1 1 2 | 42.39 |
| 2.131M | | -1 -3 1 | 42.39 |
| 2.097 | 6 | -3 0 1 | 43.10 |
| 2.063+ | 7 | 2 2 1 | 43.84 |
| 2.063+ | | 0 -2 2 | 43.84 |
| 2.012+ | 2 | -3 -2 1 | 45.02 |
| 2.012+ | | -1 2 2 | 45.02 |
| 1.959 | 7 | -2 2 0 | 46.32 |
| 1.906 | 5 | 3 2 0 | 47.67 |
| 1.893 | 1L | -1 0 3 | 48.01 |
| 1.858M | 3 | -3 1 1 | 49.00 |
| 1.858M | | -1 -1 3 | 49.00 |
| 1.835 | 4 | -1 3 1 | 49.64 |
| 1.780 | 4 | -1 1 3 | 51.28 |
| 1.7416M | 5 | -3 -3 1 | 52.50 |
| 1.7416M | | 2 3 1 | 52.50 |
| 1.7270 | 13 | 2 0 2 | 52.98 |
| 1.6852 | 1L | 3 0 1 | 54.40 |
| 1.6610 | 9 | 1 4 0 | 55.26 |
| 1.6408 | 2 | -3 -3 2 | 56.00 |

Sodium Iodate Hydrate, $\text{NaIO}_3 \cdot \text{H}_2\text{O}$

Synonym

1. Sodium iodate monohydrate

CAS registry no.

22451-04-3

Sample

The sample was crystallized by slow evaporation of an aqueous solution of NaIO_3 . The material was somewhat unstable; thus, the intensity measurements may be slightly in error.

Color

Colorless

Structure

Orthorhombic, $P2_12$ (17), $Z = 8$, assuming a density near 2.5. Indexed by use of the Visser program. The space group was assumed, based on the consideration of the absent reflections.

Lattice constants of this sample

$a = 9.065(3) \text{ \AA}$

$b = 16.632(5)$

$c = 7.638(2)$

$a/b = 0.5450$

$c/b = 0.4592$

Volume

1151.6 \AA^3

Density

(calculated) 2.491 g/cm^3

Figures of merit

$F_{30} = 18.7(0.013, 120)$

$M_{20} = 12.2$

Reference intensity

$I/I_{\text{corundum}} = 2.42(14)$

Additional pattern

1. PDF card 1-156 [Hanawalt et al., 1938]

References

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Visser, J. W. (1969). J. Appl. Crystallogr. 2, 89.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$ Internal standard Si, $a = 5.43088 \text{ \AA}$ | | | |
|--|--------------------------------------|-------|---------------------|
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 3$ | hkl | $2\theta(^{\circ})$ |
| 6.93 | 76 | 0 1 1 | 12.77 |
| 5.836 | 100 | 1 0 1 | 15.17 |
| 4.774 | 25 | 1 2 1 | 18.57 |
| 3.976 | 62 | 2 2 0 | 22.34 |
| 3.792 | 8 | 2 1 1 | 23.44 |
| 3.441 | 84 | 1 1 2 | 25.87 |
| 3.189 | 39 | 2 3 1 | 27.96 |
| 3.021 | 85 | 3 0 0 | 29.55 |
| 2.971M | 44 | 3 1 0 | 30.05 |
| 2.971M | | 1 3 2 | 30.05 |
| 2.919 | 8 | 2 0 2 | 30.60 |
| 2.890 | 19 | 1 5 1 | 30.92 |
| 2.771M | 20 | 0 6 0 | 32.28 |
| 2.771M | | 3 1 1 | 32.28 |
| 2.661 | 25 | 3 2 1 | 33.65 |
| 2.654M | 13 | 3 3 0 | 33.74 |
| 2.654M | | 1 6 0 | 33.74 |
| 2.449 | 4 | 1 0 3 | 36.67 |
| 2.391 | 12 | 2 4 2 | 37.59 |
| 2.345 | 9 | 3 1 2 | 38.35 |
| 2.328 | 3 | 3 4 1 | 38.64 |
| 2.314 | 5 | 0 3 3 | 38.88 |
| 2.279 | 23 | 3 2 2 | 39.51 |
| 2.243M | 11 | 0 6 2 | 40.17 |
| 2.243M | | 1 3 3 | 40.17 |
| 2.201M | 4 | 1 7 1 | 40.97 |
| 2.201M | | 2 1 3 | 40.97 |
| 2.144 | 4 | 2 2 3 | 42.11 |
| 2.112 | 14 | 1 4 3 | 42.78 |
| 2.023M | 6 | 4 3 1 | 44.77 |
| 2.023M | | 0 5 3 | 44.77 |
| 2.017 | 7 | 0 7 2 | 44.91 |
| 2.011 | 7 | 2 6 2 | 45.05 |
| 1.989 | 5 | 4 4 0 | 45.56 |
| 1.969 | 26 | 1 7 2 | 46.05 |
| 1.930 | 7 | 3 5 2 | 47.04 |
| 1.8976M | 4 | 4 2 2 | 47.90 |
| 1.8976M | | 0 1 4 | 47.90 |
| 1.8744 | 10 | 0 6 3 | 48.53 |
| 1.8469 | 4 | 2 5 3 | 49.30 |
| 1.8344 | 13 | 2 8 1 | 49.66 |
| 1.8196 | 4 | 4 5 1 | 50.09 |
| 1.7708M | 11 | 5 2 0 | 51.57 |
| 1.7708M | | 1 3 4 | 51.57 |
| 1.7497 | 9 | 2 1 4 | 52.24 |
| 1.7355 | 6 | 0 4 4 | 52.70 |
| 1.7218 | 7 | 2 2 4 | 53.15 |
| 1.6846 | 8 | 4 1 3 | 54.42 |

Sodium Sulfate Hydrate, $\text{Na}_2\text{S}_2\text{O}_3 \cdot 5\text{H}_2\text{O}$

Synonym

1. Sodium thiosulfate pentahydrate

CAS registry no.

10102-17-7

Sample

The sample was obtained from the Fisher Scientific Co., Fair Lawn, NJ.

Color

Colorless

Structure

Monoclinic, $P2_1/a$ (14), $Z = 4$. The structure of $\text{Na}_2\text{S}_2\text{O}_3 \cdot 5\text{H}_2\text{O}$ was determined by Taylor and Beevers [1952].

Lattice constants of this sample

$a = 7.5361(14) \text{ \AA}$

$b = 21.595(6)$

$c = 5.9503(12)$

$\beta = 103.80(2)^\circ$

$a/b = 0.3490$

$c/b = 0.2755$

Volume

940.4 \AA^3

Density

(calculated) 1.753 g/cm^3

Figure of merit

$F_{30} = 52.3(0.012, 47)$

Additional pattern

1. PDF card 13-528 [University College, Cardiff, Wales]

Reference

Taylor, P. G. and Beevers, C. A. (1952).
Acta Crystallogr. 5, 341.

$\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$

Internal standard W, $a = 3.16524 \text{ \AA}$

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 1$ | hkl | $2\theta(^\circ)$ |
|-----------------|--------------------------------------|--------|-------------------|
| 10.79 | 4 | 0 2 0 | 8.19 |
| 6.93 | 5 | 1 1 0 | 12.76 |
| 6.05 | 19 | 1 2 0 | 14.62 |
| 5.775 | 32 | 0 0 1 | 15.33 |
| 5.580 | 24 | 0 1 1 | 15.87 |
| 5.401 | 100 | 0 4 0 | 16.40 |
| 5.125 | 15 | 1 3 0 | 17.29 |
| 5.024 | 20 | -1 1 1 | 17.64 |
| 4.665 | 19 | -1 2 1 | 19.01 |
| 4.507 | 23 | 0 3 1 | 19.68 |
| 4.339 | 5 | 1 4 0 | 20.45 |
| 4.205 | 28 | -1 3 1 | 21.11 |
| 4.010 | 4 | 1 1 1 | 22.15 |
| 3.945 | 11 | 0 4 1 | 22.52 |
| 3.823 | 31 | 1 2 1 | 23.25 |
| 3.660 | 35 | 2 0 0 | 24.30 |
| 3.601 | 16 | 0 6 0 | 24.70 |
| 3.552 | 25 | 1 3 1 | 25.05 |
| 3.490 | 16 | -2 0 1 | 25.50 |
| 3.446 | 27 | -2 1 1 | 25.83 |
| 3.324 | 46 | -2 2 1 | 26.80 |
| 3.258M | 2 | 2 3 0 | 27.35 |
| 3.258M | | 1 4 1 | 27.35 |
| 3.141 | 35 | -2 3 1 | 28.39 |
| 3.031 | 2 | 2 4 0 | 29.45 |
| 2.957 | 60 | -1 6 1 | 30.20 |
| 2.911 | 35 | -1 1 2 | 30.69 |
| 2.864 | 37 | 0 1 2 | 31.20 |
| 2.843 | 34 | 1 7 0 | 31.44 |
| 2.794M | 55 | 2 5 0 | 32.01 |
| 2.794M | | 0 2 2 | 32.01 |
| 2.721M | 10 | 0 7 1 | 32.89 |
| 2.721M | | -1 3 2 | 32.89 |
| 2.648 | 1 | -1 7 1 | 33.82 |
| 2.613 | 9 | 2 3 1 | 34.29 |
| 2.586 | 8 | -2 0 2 | 34.66 |
| 2.566 | 6 | 2 6 0 | 34.94 |
| 2.548 | 6 | 0 4 2 | 35.20 |
| 2.532 | 7 | 1 8 0 | 35.42 |
| 2.506 | 13 | -2 6 1 | 35.80 |
| 2.489 | 8 | 2 4 1 | 36.06 |
| 2.451 | 47 | -3 1 1 | 36.64 |
| 2.428M | 20 | -1 5 2 | 36.99 |
| 2.428M | | 1 2 2 | 36.99 |
| 2.355 | 16 | 1 3 2 | 38.19 |
| 2.335M | 3 | -3 3 1 | 38.52 |
| 2.335M | | -2 4 2 | 38.52 |
| 2.275 | 6 | -1 6 2 | 39.58 |
| 2.263 | 10 | 1 4 2 | 39.81 |
| 2.218M | 19 | -2 5 2 | 40.65 |

Sodium Sulfate Hydrate, $\text{Na}_2\text{S}_2\text{O}_3 \cdot 5\text{H}_2\text{O}$ - (continued)

| $d(\text{\AA})$ | I^{rel} | hkl | $2\theta(^{\circ})$ |
|------------------|------------------|---------|---------------------|
| $\sigma = \pm 1$ | | | |
| 2.218M | | 0 9 1 | 40.65 |
| 2.160M | 7 | 0 10 0 | 41.78 |
| 2.160M | | 1 5 2 | 41.78 |
| 2.144 | 3 | -3 5 1 | 42.12 |
| 2.137 | 4 | -2 8 1 | 42.25 |
| 2.124 | 3 | 3 5 0 | 42.53 |
| 2.100 | 10 | -2 6 2 | 43.03 |
| 2.091 | 10 | -3 2 2 | 43.23 |
| 2.070M | 9 | 1 10 0 | 43.69 |
| 2.070M | | 1 9 1 | 43.69 |
| 2.036 | 17 | -3 6 1 | 44.47 |
| 2.007M | 7 | 2 2 2 | 45.13 |
| 2.007M | | 2 9 0 | 45.13 |
| 1.994M | 6 | 3 3 1 | 45.44 |
| 1.994M | | -1 10 1 | 45.44 |
| 1.978 | 6 | -2 9 1 | 45.85 |
| 1.951 | 3 | -1 2 3 | 46.51 |
| 1.9111+ | 11 | -1 3 3 | 47.54 |
| 1.9111+ | | -3 5 2 | 47.54 |
| 1.8961M | 3 | 0 2 3 | 47.94 |
| 1.8961M | | 1 11 0 | 47.94 |
| 1.8784 | 3 | -4 0 1 | 48.42 |
| 1.8604+ | 4 | 0 3 3 | 48.92 |
| 1.8604+ | | 2 10 0 | 48.92 |
| 1.8466M | 7 | 2 5 2 | 49.31 |
| 1.8466M | | 0 9 2 | 49.31 |
| 1.8371 | 18 | -2 10 1 | 49.58 |
| 1.8098 | 10 | 3 8 0 | 50.38 |

Strontium Bromate Hydrate, $\text{Sr}(\text{BrO}_3)_2 \cdot \text{H}_2\text{O}$

CAS registry no.
10022-52-3

Sample

The sample was made by reaction between SrCO_3 and H_2BrO_3 .

Color

Colorless

Structure

Monoclinic, $P2_1/n$ (14), $Z = 4$. The cell was obtained from axial ratios of Groth [1908], assuming $Z = 4$ and using a density of 3.778 as quoted by Groth [1908]. The space group was assumed from the peak absences.

Lattice constants of this sample

$a = 9.375(2) \text{ \AA}$
 $b = 7.6205(12)$
 $c = 8.877(2)$
 $\beta = 91.86(2)^\circ$

$a/b = 1.2302$

$c/b = 1.1648$

Volume

633.8 \AA^3

Density

(calculated) 3.788 g/cm^3

Figure of merit

$F_{30} = 35.3(0.012, 74)$

Reference intensity

$I/I_{\text{corundum}} = 2.7(2)$

Reference

Groth, P. (1908). Chemische Krystallographie II, (Wilhelm Engelmann, Leipzig, Germany) p. 113.

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 3$ | hkl | $2\theta(^\circ)$ |
|-----------------|--------------------------------------|--------|-------------------|
| 3.275 | 39 | -2 0 2 | 27.21 |
| 3.171 | 47 | 2 0 2 | 28.12 |
| 2.956 | 47 | 2 2 0 | 30.21 |
| 2.891M | 100 | 0 2 2 | 30.91 |
| 2.891M | | 3 1 0 | 30.91 |
| 2.757 | 3 | 0 1 3 | 32.45 |
| 2.484 | 5 | -2 2 2 | 36.13 |
| 2.453 | 13 | 1 3 0 | 36.60 |
| 2.445 | 13 | 0 3 1 | 36.72 |
| 2.438 | 11 | 2 2 2 | 36.83 |
| 2.409 | 2 | -2 1 3 | 37.30 |
| 2.345+ | 5 | 2 1 3 | 38.36 |
| 2.345+ | | -3 2 1 | 38.36 |
| 2.316 | 16 | 3 2 1 | 38.85 |
| 2.281 | 4 | -1 2 3 | 39.47 |
| 2.254 | 2 | 1 2 3 | 39.97 |
| 2.217 | 25 | 0 0 4 | 40.66 |
| 2.188 | 8 | -4 1 1 | 41.23 |
| 2.173 | 4 | -2 3 1 | 41.52 |
| 2.156M | 8 | 4 1 1 | 41.86 |
| 2.156M | | 2 3 1 | 41.86 |
| 2.138 | 3 | 1 3 2 | 42.23 |
| 2.099M | 6 | -3 1 3 | 43.07 |
| 2.099M | | 3 2 2 | 43.07 |
| 2.063 | 1 | 1 1 4 | 43.85 |
| 2.044 | 2 | 4 0 2 | 44.27 |
| 1.9160+ | 4 | 2 1 4 | 47.41 |
| 1.9160+ | | 0 2 4 | 47.41 |
| 1.8931 | 5 | -3 2 3 | 48.02 |
| 1.8237 | 9 | 1 4 1 | 49.97 |
| 1.8189 | 11 | 5 1 0 | 50.11 |
| 1.8145 | 10 | -3 3 2 | 50.24 |
| 1.7876 | 19 | 3 3 2 | 51.05 |
| 1.7651 | 10 | 2 4 0 | 51.75 |
| 1.7591 | 10 | 4 1 3 | 51.94 |
| 1.7509 | 11 | 0 4 2 | 52.20 |
| 1.7343+ | 7 | 3 1 4 | 52.74 |
| 1.7343+ | | -2 4 1 | 52.74 |
| 1.7020 | 9 | -5 1 2 | 53.82 |
| 1.6832 | 1 | 4 3 1 | 54.47 |
| 1.6649 | 7 | 5 1 2 | 55.12 |
| 1.6514 | 2 | -1 3 4 | 55.61 |
| 1.6341M | 4 | 4 2 3 | 56.25 |
| 1.6341M | | 2 4 2 | 56.25 |
| 1.6043 | 2 | -3 4 1 | 57.39 |
| 1.5921 | 3 | 4 3 2 | 57.87 |
| 1.5829 | 2 | -1 4 3 | 58.24 |
| 1.5617M | 2 | 2 3 4 | 59.11 |
| 1.5617M | | 6 0 0 | 59.11 |
| 1.5077+ | 7 | 2 2 5 | 61.45 |
| 1.5077+ | | 5 3 0 | 61.45 |
| 1.4774 | 2 | 4 4 0 | 62.85 |

| $\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}; \text{ temp. } 25 \pm 1^\circ \text{C}$ | | | |
|---|--------------------------------------|--------|-------------------|
| Internal standard W, $a = 3.16524 \text{ \AA}$ | | | |
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 3$ | hkl | $2\theta(^\circ)$ |
| 5.91 | 6 | 1 1 0 | 14.97 |
| 5.779 | 33 | 0 1 1 | 15.32 |
| 4.687 | 4 | 2 0 0 | 18.92 |
| 4.434 | 23 | 0 0 2 | 20.01 |
| 3.836 | 12 | 0 1 2 | 23.17 |
| 3.811 | 32 | 0 2 0 | 23.32 |
| 3.681 | 6 | -2 1 1 | 24.16 |
| 3.586 | 31 | -1 1 2 | 24.81 |
| 3.515 | 20 | 1 1 2 | 25.32 |
| 3.293 | 32 | -1 2 1 | 27.06 |

Strontium Chromium Oxide, SrCr₂O₇

Synonym

1. Strontium dichromate

Sample

The sample was prepared by heating SrCr₂O₇·3H₂O at 130 °C for 18 hours, followed by heating at 150 °C for 24 hours.

Color

Deep orange yellow

Structure

Tetragonal, P₄₂/nmc (137), Z = 8, isostructural with PbCr₂O₇. The structure of SrCr₂O₇ was determined by Wilhelmi [1967].

Lattice constants of this sample

a = 11.1925(7) Å

c = 9.4833(11)

c/a = 0.8473

Volume

1188.0 Å³

Density

(calculated) 3.395 g/cm³

Figure of merit

F₃₀ = 72.4(0.010,41)

Reference intensity

I/I_{corundum} = 2.35(8)

Additional pattern

1. PDF card 20-1191 [Wilhelmi, 1967]

Reference

Wilhelmi, K.-A. (1967). Ark. Kemi 26, 149.

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C Internal standard Si, a = 5.43088 Å | | | | |
|--|----------------------------|-------|-------|--|
| d(Å) | I ^{rel} σ = ±2 | hkl | 2θ(°) | |
| 7.91 | 2 | 1 1 0 | 11.17 | |
| 7.24 | 2 | 1 0 1 | 12.22 | |
| 5.601 | 5 | 2 0 0 | 15.81 | |
| 4.739 | 3 | 0 0 2 | 18.71 | |
| 4.423 | 11 | 2 1 1 | 20.06 | |
| 4.070 | 4 | 1 1 2 | 21.82 | |
| 3.955 | 2 | 2 2 0 | 22.46 | |
| 3.619 | 68 | 2 0 2 | 24.58 | |
| 3.538 | 4 | 3 1 0 | 25.15 | |
| 3.474 | 25 | 3 0 1 | 25.62 | |
| 3.443 | 5 | 2 1 2 | 25.86 | |
| 3.315 | 100 | 3 1 1 | 26.87 | |
| 3.040M | 32 | 1 0 3 | 29.36 | |
| 3.040M | | 2 2 2 | 29.36 | |
| 2.950 | 15 | 3 2 1 | 30.27 | |
| 2.931 | 11 | 3 0 2 | 30.47 | |
| 2.836 | 3 | 3 1 2 | 31.52 | |
| 2.796 | 2 | 4 0 0 | 31.98 | |
| 2.751 | 1 | 2 0 3 | 32.52 | |
| 2.673 | 2 | 2 1 3 | 33.50 | |
| 2.636 | 2 | 3 3 0 | 33.98 | |
| 2.609 | 1 | 4 1 1 | 34.34 | |
| 2.596 | 2 | 3 2 2 | 34.52 | |
| 2.503 | 9 | 4 2 0 | 35.85 | |
| 2.420 | 7 | 4 2 1 | 37.12 | |
| 2.413 | 9 | 3 0 3 | 37.24 | |
| 2.357M | 11 | 3 1 3 | 38.15 | |
| 2.357M | | 4 1 2 | 38.15 | |
| 2.305 | 6 | 3 3 2 | 39.04 | |
| 2.2145M | 12 | 3 2 3 | 40.71 | |
| 2.2145M | | 4 2 2 | 40.71 | |
| 2.1944 | 7 | 5 1 0 | 41.10 | |
| 2.1787 | 15 | 4 3 1 | 41.41 | |
| 2.1388 | 3 | 5 1 1 | 42.22 | |
| 2.0948 | 1 | 4 0 3 | 43.15 | |
| 2.0304 | 29 | 5 2 1 | 44.59 | |
| 2.0011 | 3 | 3 0 4 | 45.28 | |
| 1.9779 | 2 | 4 4 0 | 45.84 | |
| 1.9195 | 8 | 5 3 0 | 47.32 | |
| 1.8835 | 1 | 3 2 4 | 48.28 | |
| 1.8813 | 2 | 5 3 1 | 48.34 | |
| 1.8654 | 8 | 6 0 0 | 48.78 | |
| 1.8264M | 13 | 4 3 3 | 49.89 | |
| 1.8264M | | 4 4 2 | 49.89 | |
| 1.8088 | 1 | 4 0 4 | 50.41 | |

Strontium Chromium Oxide, SrCr_2O_7 - (continued)

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 2$ | hkl | $2\theta(^{\circ})$ |
|-----------------|--------------------------------------|-------|---------------------|
| 1.8038 | 2 | 5 1 3 | 50.56 |
| 1.7795 | 6 | 5 3 2 | 51.30 |
| 1.7635 | 5 | 3 3 4 | 51.80 |
| 1.7367M | 2 | 5 2 3 | 52.66 |
| 1.7367M | | 6 0 2 | 52.66 |
| 1.7203 | 4 | 4 2 4 | 53.20 |
| 1.6909 | 4 | 3 0 5 | 54.20 |
| 1.6585 | 2 | 6 2 2 | 55.35 |
| 1.6432 | 1 | 6 3 1 | 55.91 |
| 1.6185 | 4 | 3 2 5 | 56.84 |
| 1.5904 | 1 | 6 1 3 | 57.94 |
| 1.5829 | 2 | 7 1 0 | 58.24 |
| 1.5770 | 2 | 7 0 1 | 58.48 |
| 1.5547 | 1 | 4 1 5 | 59.40 |
| 1.5502 | 1L | 1 1 6 | 59.59 |
| 1.5316 | 1L | 6 4 1 | 60.39 |
| 1.5175 | 3 | 7 2 1 | 61.01 |
| 1.5150 | 1L | 7 0 2 | 61.12 |
| 1.5015 | 1 | 7 1 2 | 61.73 |
| 1.4699 | 2 | 7 3 0 | 63.21 |
| 1.4524 | 6 | 7 3 1 | 64.06 |

Strontium Chromium Oxide Hydrate, $\text{SrCr}_2\text{O}_7 \cdot 3\text{H}_2\text{O}$

Synonym

1. Strontium dichromate trihydrate

Sample

The sample was prepared by adding SrCrO_4 to a saturated solution of CrO_3 . Large red crystals formed slowly.

Color

Unground, deep reddish brown. Ground, deep orange.

Structure

Monoclinic, $P2_1/c$ (14), $Z = 4$. The crystallographic information was obtained on a single crystal diffractometer by V. Himes. The cell parameters were confirmed by the Visser program [1969] and by axial ratios given by Groth [1908], assuming $Z = 4$ and a density near 2.6.

Lattice constants of this sample

$a = 8.3583(12) \text{ \AA}$
 $b = 14.023(2)$
 $c = 7.574(2)$
 $\beta = 91.95(2)^\circ$

$a/b = 0.5960$
 $c/b = 0.5401$

Volume

887.22 \AA^3

Density

(calculated) 2.678 g/cm^3

Figures of merit

$F_{30} = 74.8 (0.010, 40)$
 $M_{20} = 38.4$

Reference intensity

$I/I_{\text{corundum}} = 1.04(5)$

References

Groth, P. (1908). *Chemische Krystallographie* II (Wilhelm Engelmann, Leipzig, Germany) p. 593.
 Visser, J. W. (1969). *J. Appl. Crystallogr.* 2, 89.

| CuK α_1 $\lambda = 1.540598 \overset{\circ}{\text{\AA}}$; temp. 25 \pm 1 $^{\circ}\text{C}$ | | | | |
|---|------------------|--------|---------------------|--|
| Internal standard Si, a = 5.43088 $\overset{\circ}{\text{\AA}}$ | | | | |
| $d(\overset{\circ}{\text{\AA}})$ | I^{rel} | hkl | $2\theta(^{\circ})$ | |
| $\sigma = \pm 3$ | | | | |
| 8.35 | 31 | 1 0 0 | 10.59 | |
| 7.18 | 9 | 1 1 0 | 12.31 | |
| 7.02 | 8 | 0 2 0 | 12.60 | |
| 6.67 | 4 | 0 1 1 | 13.27 | |
| 5.368 | 9 | 1 2 0 | 16.50 | |
| 5.286 | 25 | -1 1 1 | 16.76 | |
| 5.142M | 10 | 0 2 1 | 17.23 | |
| 5.142M | | 1 1 1 | 17.23 | |
| 4.425 | 21 | -1 2 1 | 20.05 | |
| 4.337 | 20 | 1 2 1 | 20.46 | |
| 4.178 | 100 | 2 0 0 | 21.25 | |
| 4.079 | 23 | 1 3 0 | 21.77 | |
| 4.001 | 68 | 2 1 0 | 22.20 | |
| 3.980 | 70 | 0 3 1 | 22.32 | |
| 3.784 | 45 | 0 0 2 | 23.49 | |
| 3.652 | 25 | 0 1 2 | 24.35 | |
| 3.614 | 25 | -1 3 1 | 24.61 | |
| 3.589M | 10 | 2 2 0 | 24.79 | |
| 3.589M | | -2 1 1 | 24.79 | |
| 3.504 | 45 | 0 4 0 | 25.40 | |
| 3.388 | 21 | -1 1 2 | 26.28 | |
| 3.307 | 4 | 1 1 2 | 26.94 | |
| 3.282 | 3 | -2 2 1 | 27.15 | |
| 3.230 | 17 | 1 4 0 | 27.59 | |
| 3.208 | 35 | 2 2 1 | 27.79 | |
| 3.181 | 7 | 0 4 1 | 28.03 | |
| 3.128 | 4 | -1 2 2 | 28.51 | |
| 3.061 | 3 | 1 2 2 | 29.15 | |
| 2.987 | 13 | -1 4 1 | 29.89 | |
| 2.958 | 14 | 1 4 1 | 30.19 | |
| 2.907 | 13 | -2 3 1 | 30.73 | |
| 2.856M | 15 | 2 3 1 | 31.29 | |
| 2.856M | | -2 0 2 | 31.29 | |
| 2.785 | 20 | 3 0 0 | 32.11 | |
| 2.752 | 7 | 1 3 2 | 32.51 | |
| 2.731 | 6 | 3 1 0 | 32.76 | |
| 2.706 | 20 | 2 1 2 | 33.08 | |
| 2.686 | 9 | 2 4 0 | 33.33 | |
| 2.657 | 10 | 1 5 0 | 33.70 | |
| 2.597 | 15 | -3 1 1 | 34.51 | |
| 2.567 | 13 | 2 2 2 | 34.92 | |
| 2.541 | 9 | 3 1 1 | 35.29 | |
| 2.500 | 3 | 1 5 1 | 35.89 | |
| 2.473M | 7 | -1 4 2 | 36.30 | |
| 2.473M | | -3 2 1 | 36.30 | |

Strontium Chromium Oxide Hydrate, $\text{SrCr}_2\text{O}_7 \cdot 3\text{H}_2\text{O}$ - (continued)

| $d(\text{\AA})$ | I^{rel} | hkl | $2\theta(^{\circ})$ |
|------------------|------------------|--------|---------------------|
| $\sigma = \pm 3$ | | | |
| 2.425 | 20 | 3 2 1 | 37.04 |
| 2.393 | 30 | 3 3 0 | 37.56 |
| 2.359 | 3 | 1 1 3 | 38.11 |
| 2.338 | 3 | 0 6 0 | 38.48 |
| 2.302M | 9 | -1 2 3 | 39.10 |
| 2.302M | | -3 3 1 | 39.10 |
| 2.263M | 1 | 1 2 3 | 39.80 |
| 2.263M | | 3 3 1 | 39.80 |
| 2.233 | 4 | 0 6 1 | 40.36 |
| 2.212M | 5 | 2 5 1 | 40.75 |
| 2.212M | | -2 4 2 | 40.75 |
| 2.186 | 4 | -1 5 2 | 41.26 |
| 2.1662+ | 25 | 2 4 2 | 41.66 |
| 2.1662+ | | -2 1 3 | 41.66 |
| 2.1036M | 16 | 3 2 2 | 42.96 |
| 2.1036M | | 2 1 3 | 42.96 |
| 2.0879 | 10 | 4 0 0 | 43.30 |
| 2.0648 | 2 | 4 1 0 | 43.81 |
| 2.0492M | 13 | -3 3 2 | 44.16 |
| 2.0492M | | 0 4 3 | 44.16 |
| 2.0103 | 12 | -4 1 1 | 45.06 |
| 2.0028M | 21 | -1 4 3 | 45.24 |
| 2.0028M | | 4 2 0 | 45.24 |
| 1.9767M | 32 | 1 4 3 | 45.87 |
| 1.9767M | | 3 5 0 | 45.87 |
| 1.9622 | 5 | 2 6 1 | 46.23 |
| 1.9376M | 24 | 0 7 1 | 46.85 |
| 1.9376M | | 2 3 3 | 46.85 |

Thiosemicarbazide, CH₅N₃S

Synonym

1. Hydrazinecarbothioamide

CAS registry no.

79-19-6

Sample

The sample was obtained from J. T. Baker Co., Phillipsburg, NJ. It was re-crystallized from ethanol.

Color

Colorless

Structure

Triclinic, $P\bar{1}$ (2), $Z = 2$. The structure was determined by Andreetti et al. [1970].

Lattice constants of this sample

$a = 6.0266(12) \text{ \AA}$

$b = 7.327(2)$

$c = 4.9353(15)$

$\alpha = 103.00(2)^\circ$

$\beta = 96.33(2)$

$\gamma = 77.21(2)$

$a/b = 0.8225$

$c/b = 0.6736$

Volume

206.65 \AA^3

Density

(calculated) 1.465 g/cm^3

Figure of merit

$F_{30} = 40.9(0.015, 50)$

Reference intensity

$I/I_{\text{corundum}} = 2.56(11)$

Additional pattern

1. PDF card 24-1952 [Institute of Physics, University College, Cardiff, Wales]

Reference

Andreetti, G. D., Domiano, P., Gasparri, G. F., Nardelli, M., and Sgarabotto, P. (1970). Acta Crystallogr. **B26**, 1005.

| CuK α_1 $\lambda = 1.540598 \overset{\circ}{\text{\AA}}$; temp. 25 \pm 1 $^{\circ}\text{C}$ | | | | | |
|---|------------------|-----|----|---|----------------------|
| Internal standard W, a = 3.16524 $\overset{\circ}{\text{\AA}}$ | | | | | |
| $d(\overset{\circ}{\text{\AA}})$ | I^{rel} | hkl | | | 2 $\theta(^{\circ})$ |
| $\sigma = \pm 2$ | | | | | |
| 5.86 | 5 | 1 | 0 | 0 | 15.11 |
| 5.021 | 18 | 1 | 1 | 0 | 17.65 |
| 4.797 | 13 | 0 | 0 | 1 | 18.48 |
| 4.399 | 5 | 0 | -1 | 1 | 20.17 |
| 4.100 | 4 | -1 | 1 | 0 | 21.66 |
| 3.619 | 36 | 0 | 1 | 1 | 24.58 |
| 3.497 | 11 | 0 | 2 | 0 | 25.45 |
| 3.309 | 1 | 1 | 2 | 0 | 26.92 |
| 3.245 | 11 | 1 | -1 | 1 | 27.46 |
| 3.163 | 100 | 1 | 1 | 1 | 28.19 |
| 3.082 | 7 | -1 | -2 | 1 | 28.95 |
| 3.008 | 8 | -1 | 1 | 1 | 29.68 |
| 2.931 | 6 | 2 | 0 | 0 | 30.47 |
| 2.767 | 1L | -1 | 2 | 0 | 32.33 |
| 2.685 | 1 | -2 | -1 | 1 | 33.35 |
| 2.582 | 1 | 0 | 2 | 1 | 34.71 |
| 2.548 | 2 | 1 | -2 | 1 | 35.19 |
| 2.527 | 4 | -2 | 1 | 0 | 35.49 |
| 2.512 | 1 | 2 | 2 | 0 | 35.71 |
| 2.472 | 3 | 1 | 2 | 1 | 36.31 |
| 2.437M | 2 | -2 | -2 | 1 | 36.86 |
| 2.437M | | 2 | 0 | 1 | 36.86 |
| 2.333 | 2 | 1 | 3 | 0 | 38.56 |
| 2.291 | 1L | 0 | -3 | 1 | 39.29 |
| 2.271M | 1L | -1 | 0 | 2 | 39.66 |
| 2.271M | | -1 | 2 | 1 | 39.66 |
| 2.202M | 2 | 0 | -2 | 2 | 40.95 |
| 2.202M | | -1 | -2 | 2 | 40.95 |
| 2.173 | 2 | 1 | 0 | 2 | 41.52 |
| 2.143 | 1 | 1 | -1 | 2 | 42.13 |
| 2.138 | 1L | 0 | 1 | 2 | 42.23 |
| 2.051 | 2 | -2 | 2 | 0 | 44.13 |
| 2.037 | 1 | 2 | 3 | 0 | 44.44 |
| 2.008 | 2 | -2 | -1 | 2 | 45.11 |
| 1.990 | 1 | 3 | 1 | 0 | 45.54 |
| 1.985 | 2 | 1 | -3 | 1 | 45.66 |
| 1.945M | 1 | 1 | -2 | 2 | 46.66 |
| 1.945M | | 0 | 3 | 1 | 46.66 |
| 1.929 | 1L | 1 | 3 | 1 | 47.06 |
| 1.925 | 1L | -3 | -1 | 1 | 47.18 |

Thiosemicarbazide, CH₅N₃S - (continued)

| d(Å) | I ^{rel} | hkl | 2θ(°) |
|---------|------------------|---------|-------|
| σ = ±2 | | | |
| 1.877M | 1L | 0 -3 2 | 48.47 |
| 1.877M | | 3 2 0 | 48.47 |
| 1.859 | 2 | -3 -2 1 | 48.95 |
| 1.836 | 1 | -2 2 1 | 49.61 |
| 1.811 | 1 | 0 2 2 | 50.35 |
| 1.8025 | 1 | 2 0 2 | 50.60 |
| 1.7906 | 1 | -3 1 0 | 50.96 |
| 1.7724M | 2 | 3 0 1 | 51.52 |
| 1.7724M | | -1 3 1 | 51.52 |
| 1.7594+ | 4 | -2 -3 2 | 51.93 |
| 1.7594+ | | 1 2 2 | 51.93 |
| 1.7315 | 2 | 2 1 2 | 52.83 |
| 1.7034 | 1L | -1 2 2 | 53.77 |
| 1.6907M | 1L | -2 -4 1 | 54.21 |
| 1.6907M | | -3 -3 1 | 54.21 |
| 1.6741M | 1 | 3 -1 1 | 54.79 |
| 1.6741M | | 3 3 0 | 54.79 |
| 1.6541 | 1L | 3 2 1 | 55.51 |
| 1.6219M | 1 | -1 -1 3 | 56.71 |
| 1.6219M | | 2 -2 2 | 56.71 |

Thiourea, CH₄N₂S

Synonym

1. Thiocarbamide

CAS registry no.

62-56-6

Sample

The sample was obtained from J. T. Baker Chemical Co., Phillipsburg, NJ. It was recrystallized from ethanol.

Color

Colorless

Structure

Orthorhombic, Pnma (62), Z = 4. The structure was first determined by Demeny and Nitta, [1928]. It was later refined by Truter [1957].

Lattice constants of this sample

a = 7.6644(12) Å

b = 8.5591(12)

c = 5.4925(8)

a/b = 0.8955

c/b = 0.6417

Volume

360.31 Å³

Density

(calculated) 1.403 g/cm³

Figure of merit

F₃₀ = 66.3(0.009,49)

Reference intensity

I/I_{corundum} = 0.91(3)

Additional pattern

1. PDF card 9-790 [Morse and Baun, Wright Patterson Air Force Base, Ohio]

References

Demeny, L. and Nitta, I. (1928). Bull. Chem. Soc. Japan 3, 128.

Truter, M. R. (1957). Acta Crystallogr. 10, 786.

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C | | | | |
|---|------------------|-------|-------|--|
| Internal standard W, a = 3.16524 Å | | | | |
| d(Å) | I ^{rel} | hkl | 2θ(°) | |
| σ = ±2 | | | | |
| 4.624 | 9 | 0 1 1 | 19.18 | |
| 4.467 | 70 | 1 0 1 | 19.86 | |
| 4.279 | 100 | 0 2 0 | 20.74 | |
| 3.834 | 61 | 2 0 0 | 23.18 | |
| 3.498 | 53 | 2 1 0 | 25.44 | |
| 3.142 | 65 | 2 0 1 | 28.38 | |
| 3.089 | 66 | 1 2 1 | 28.88 | |
| 2.951 | 24 | 2 1 1 | 30.26 | |
| 2.855 | 45 | 2 2 0 | 31.31 | |
| 2.747 | 8 | 0 0 2 | 32.57 | |
| 2.532M | 28 | 2 2 1 | 35.43 | |
| 2.532M | | 0 3 1 | 35.43 | |
| 2.475 | 31 | 1 1 2 | 36.26 | |
| 2.405 | 1 | 1 3 1 | 37.36 | |
| 2.317 | 9 | 3 0 1 | 38.83 | |
| 2.2885 | 3 | 2 3 0 | 39.34 | |
| 2.1598 | 7 | 2 1 2 | 41.79 | |
| 2.1393 | 2 | 0 4 0 | 42.21 | |
| 2.1116 | 5 | 2 3 1 | 42.79 | |
| 2.0369 | 8 | 3 2 1 | 44.44 | |
| 1.9291 | 14 | 1 4 1 | 47.07 | |
| 1.9164M | 5 | 4 0 0 | 47.40 | |
| 1.9164M | | 1 3 2 | 47.40 | |
| 1.8683 | 9 | 2 4 0 | 48.70 | |
| 1.8271 | 8 | 3 1 2 | 49.87 | |
| 1.7902 | 7 | 0 1 3 | 50.97 | |
| 1.7695M | 11 | 4 1 1 | 51.61 | |
| 1.7695M | | 2 4 1 | 51.61 | |
| 1.7487 | 3 | 4 2 0 | 52.27 | |
| 1.7135 | 1 | 3 2 2 | 53.43 | |
| 1.6883 | 1 | 0 4 2 | 54.29 | |
| 1.6665 | 1L | 4 2 1 | 55.06 | |
| 1.6440 | 4 | 1 2 3 | 55.88 | |
| 1.6346 | 2 | 0 5 1 | 56.23 | |
| 1.6219 | 3 | 2 1 3 | 56.71 | |
| 1.5716M | 3 | 3 4 1 | 58.70 | |
| 1.5716M | | 4 0 2 | 58.70 | |
| 1.5643 | 4 | 3 3 2 | 59.00 | |

Tin Chloride Hydrate, $\text{SnCl}_2 \cdot 2\text{H}_2\text{O}$

Synonym

1. Stannous chloride dihydrate

CAS registry no.

10025-69-1

Sample

The sample was obtained from Fisher Scientific Co., Fair Lawn, NJ.

Color

Colorless

Structure

Monoclinic, $P2_1/c$ (14), $Z = 4$. The structure of $\text{SnCl}_2 \cdot 2\text{H}_2\text{O}$ was determined by Grdenic and Kamenar [1960].

Lattice constants of this sample

$a = 9.318(3) \text{ \AA}$

$b = 7.2571(14)$

$c = 8.973(2)$

$\beta = 114.89(2)^\circ$

$a/b = 1.2840$

$c/b = 1.2365$

Volume

550.4 \AA^3

Density

(calculated) 2.723 g/cm^3

Figure of merit

$F_{30} = 49.4 (0.012, 49)$

Reference intensity

$I/I_{\text{corundum}} = 1.50(2)$

Additional pattern

1. PDF card 20-1292 [University of Leeds, Leeds, England]

Reference

Grdenic, D. and Kamenar, B. (1960). Proc. Chem. Soc. 1960, 312.

| CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$ | | | |
|---|--------------------------------------|--------|-------------------|
| Internal standard Si, $a = 5.43088 \text{ \AA}$ | | | |
| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 8$ | hkl | $2\theta(^\circ)$ |
| 8.43 | 59 | 1 0 0 | 10.48 |
| 5.511 | 100 | 1 1 0 | 16.07 |
| 5.414 | 8 | 0 1 1 | 16.36 |
| 5.279 | 4 | -1 1 1 | 16.78 |
| 4.483 | 1 | -1 0 2 | 19.79 |
| 4.227 | 11 | 2 0 0 | 21.00 |
| 4.068M | 19 | 1 1 1 | 21.83 |
| 4.068M | | 0 0 2 | 21.83 |
| 3.902 | 4 | -2 1 1 | 22.77 |
| 3.810 | 53 | -1 1 2 | 23.33 |
| 3.655 | 81 | 2 1 0 | 24.33 |
| 3.628 | 13 | 0 2 0 | 24.52 |
| 3.551 | 12 | 0 1 2 | 25.06 |
| 3.402 | 43 | -2 1 2 | 26.17 |
| 3.334 | 8 | 1 2 0 | 26.72 |
| 3.181 | 8 | 1 0 2 | 28.03 |
| 2.953 | 6 | 2 1 1 | 30.24 |
| 2.912 | 5 | 1 1 2 | 30.68 |
| 2.819M | 28 | -1 2 2 | 31.72 |
| 2.819M | | 3 0 0 | 31.72 |
| 2.754M | 20 | -3 1 2 | 32.49 |
| 2.754M | | 2 2 0 | 32.49 |
| 2.709 | 60 | 0 2 2 | 33.04 |
| 2.642 | 34 | -2 2 2 | 33.90 |
| 2.627 | 22 | 3 1 0 | 34.10 |
| 2.541 | 6 | 0 1 3 | 35.29 |
| 2.461 | 14 | 2 0 2 | 36.48 |
| 2.420 | 4 | -3 1 3 | 37.12 |
| 2.392 | 19 | 1 2 2 | 37.57 |
| 2.327 | 24 | 1 3 0 | 38.67 |
| 2.318M | 25 | 0 3 1 | 38.82 |
| 2.318M | | -4 0 2 | 38.82 |
| 2.303 | 25 | -3 2 2 | 39.09 |
| 2.253 | 2 | 3 1 1 | 39.99 |
| 2.238 | 10 | -2 0 4 | 40.26 |
| 2.225 | 2 | 3 2 0 | 40.51 |
| 2.206M | 2 | -4 1 2 | 40.87 |
| 2.206M | | 1 1 3 | 40.87 |
| 2.171 | 3 | 1 3 1 | 41.57 |
| 2.138 | 7 | -2 1 4 | 42.24 |
| 2.130M | 20 | -3 0 4 | 42.41 |
| 2.130M | | -1 3 2 | 42.41 |
| 2.113 | 4 | 4 0 0 | 42.75 |
| 2.100 | 25 | 2 3 0 | 43.04 |
| 2.079 | 4 | 0 3 2 | 43.50 |
| 2.048 | 12 | -2 3 2 | 44.18 |
| 2.035M | 3 | 2 2 2 | 44.49 |
| 2.035M | | 0 0 4 | 44.49 |
| 1.960 | 10 | 0 1 4 | 46.29 |
| 1.953M | 12 | -4 2 2 | 46.47 |

Tin Chloride Hydrate, $\text{SnCl}_2 \cdot 2\text{H}_2\text{O}$ - (continued)

| $d(\text{\AA})$ | I^{rel} $\sigma = \pm 8$ | hkl | $2\theta(^{\circ})$ |
|-----------------|--------------------------------------|--------|---------------------|
| 1.953M | | 1 2 3 | 46.47 |
| 1.924M | 4 | -4 0 4 | 47.19 |
| 1.924M | | 1 3 2 | 47.19 |
| 1.905M | 9 | -3 3 1 | 47.71 |
| 1.905M | | -2 2 4 | 47.71 |
| 1.894 | 10 | 3 1 2 | 47.99 |
| 1.8766M | 4 | -1 3 3 | 48.47 |
| 1.8766M | | 2 1 3 | 48.47 |
| 1.8618M | 8 | -4 1 4 | 48.88 |
| 1.8618M | | -4 2 3 | 48.88 |
| 1.8357M | 9 | -3 2 4 | 49.62 |
| 1.8357M | | 3 3 0 | 49.62 |
| 1.8264 | 17 | 4 2 0 | 49.89 |
| 1.8142 | 17 | 0 4 0 | 50.25 |
| 1.8061M | 14 | 0 3 3 | 50.49 |
| 1.8061M | | -5 1 2 | 50.49 |
| 1.7734 | 8 | 1 4 0 | 51.49 |
| 1.7610M | 6 | -3 3 3 | 51.88 |
| 1.7610M | | -5 1 1 | 51.88 |
| 1.7246 | 8 | 2 3 2 | 53.06 |

Zirconium Silicide, ZrSi₂

CAS registry no.
12039-90-6

Sample

The sample was prepared at NBS by R. F. Walker and S. Y. Holley. The sample had a small amount of ZrO₂ and Si present.

Major impurities

>1% Hf; 0.1 to 1.0 % Al; 0.01 to 0.1% each Fe, Ni, and Ti; and 0.001 to 0.01% each Ca, Cr, and Mn.

Structure

Orthorhombic, Cmc₂m (63), Z = 4 [Seyfarth, 1928]. The structure was redetermined by Schachner et al. [1954] and by Vaughn and Bracuti [1958].

Lattice constants of this sample

a = 3.6958(3) Å
b = 14.7514(9)
c = 3.6654(3)

a/b = 0.2505
c/b = 0.2485

Volume

199.83 Å³

Density

(calculated) 4.899 g/cm³

Figure of merit

F₃₀ = 81.8(0.009,40)

Additional pattern

1. PDF card 10-236 [Cotter et al., 1956].

References

- Cotter, P. G., Kohn, J. A., and Potter, R. A. (1956). J. Amer. Ceram. Soc. 39, 11.
Schachner, H., Nowotny, H., and Kudielka, H. (1954). Monatsh. Chem. 85, 1140.
Seyfarth, H. (1928). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 67, 295.
Vaughn, P. A. and Bracuti, A. (1958). Diss. Abstr. B. 19, 1217.

| CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C Internal standard W, a = 3.16524 Å | | | |
|---|----------------------------|--------|-------|
| d(Å) | I ^{rel} σ = ±2 | hkl | 2θ(°) |
| 7.37 | 4 | 0 2 0 | 12.00 |
| 3.685 | 9 | 0 4 0 | 24.13 |
| 3.586 | 15 | 1 1 0 | 24.81 |
| 3.283 | 32 | 0 2 1 | 27.14 |
| 2.954 | 15 | 1 3 0 | 30.23 |
| 2.601 | 1 | 0 4 1 | 34.46 |
| 2.564 | 10 | 1 1 1 | 34.97 |
| 2.458 | 15 | 0 6 0 | 36.53 |
| 2.300 | 100 | 1 3 1 | 39.14 |
| 2.0417 | 14 | 0 6 1 | 44.33 |
| 1.9518 | 1 | 1 5 1 | 46.49 |
| 1.8480 | 11 | 2 0 0 | 49.27 |
| 1.8434 | 7 | 0 8 0 | 49.40 |
| 1.8330 | 14 | 0 0 2 | 49.70 |
| 1.7782 | 1L | 0 2 2 | 51.34 |
| 1.6519 | 2 | 2 4 0 | 55.59 |
| 1.6473 | 7 | 0 8 1 | 55.76 |
| 1.6381 | 7 | 1 7 1 | 56.10 |
| 1.6322 | 6 | 1 1 2 | 56.32 |
| 1.6102 | 7 | 2 2 1 | 57.16 |
| 1.5576 | 4 | 1 3 2 | 59.28 |
| 1.4982 | 6 | 1 9 0 | 61.88 |
| 1.4772 | 4 | 2 6 0 | 62.86 |
| 1.4692 | 5 | 0 6 2 | 63.24 |
| 1.4346 | 6 | 1 5 2 | 64.95 |
| 1.3867 | 2 | 1 9 1 | 67.49 |
| 1.3704 | 6 | 2 6 1 | 68.40 |
| 1.3050 | 1 | 2 8 0 | 72.35 |
| 1.3016 | 5 | 2 0 2 | 72.57 |
| 1.2603 | 1 | 1 11 0 | 75.35 |
| 1.2296M | 3 | 2 8 1 | 77.58 |
| 1.2296M | | 0 12 0 | 77.58 |
| 1.2269 | 3 | 2 4 2 | 77.78 |
| 1.2051 | 1 | 0 2 3 | 79.46 |
| 1.1923 | 2 | 1 11 1 | 80.49 |
| 1.1655 | 1 | 0 12 1 | 82.74 |
| 1.1641 | 1 | 3 1 1 | 82.86 |
| 1.1602M | 3 | 1 9 2 | 83.20 |
| 1.1602M | | 0 4 3 | 83.20 |
| 1.1502 | 2 | 2 6 2 | 84.09 |
| 1.1361 | 6 | 3 3 1 | 85.38 |
| 1.1291 | 4 | 1 3 3 | 86.04 |
| 1.0998 | 1L | 2 10 1 | 88.92 |
| 1.0942 | 1L | 0 6 3 | 89.50 |
| 1.0849 | 1L | 1 13 0 | 90.47 |
| 1.0631 | 1 | 2 8 2 | 92.87 |
| 1.0538 | 1 | 0 14 0 | 93.94 |
| 1.0386 | 1 | 1 11 2 | 95.75 |

INORGANIC NAMES

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|--|-----------------|------|--|-----------------|------|
| Aluminum, Al | 1 | 11 | Ammonium aluminum selenate hydrate, NH ₄ Al(SeO ₄) ₂ ·12H ₂ O | 9m | 6 |
| Aluminum antimony, AlSb | 4 | 72 | Ammonium aluminum sulfate, NH ₄ Al(SO ₄) ₂ | 10m | 5 |
| Aluminum bismuth oxide, Al ₄ Bi ₂ O ₉ .. | 11m | 5 | Ammonium aluminum sulfate hydrate (tschermigite), NH ₄ Al(SO ₄) ₂ ·12H ₂ O | 6 | 3 |
| Aluminum borate, Al ₁₈ B ₄ O ₃₃ | 17m | 5 | Ammonium azide, NH ₄ N ₃ | 9 | 4 |
| Aluminum chloride, AlCl ₃ | 9m | 61 | Ammonium beryllium fluoride, (NH ₄) ₂ BeF ₄ | 3m | 5 |
| Aluminum chloride hydrate (chloraluminite), AlCl ₃ ·6H ₂ O | 7 | 3 | Ammonium borate hydrate, NH ₄ B ₅ O ₈ ·4H ₂ O | 17m | 7 |
| Aluminum copper, Al ₄ Cu ₉ | 11m | 79 | Ammonium boron fluoride, NH ₄ BF ₄ ... | 3m | 6 |
| Aluminum fluoride hydroxide silicate, topaz, Al ₂ (F,OH) ₂ SiO ₄ | 1m | 4 | Ammonium bromide, NH ₄ Br | 2 | 49 |
| Aluminum iron antimony oxide, bahianite, Al _{5.66} Fe _{0.09} Sb _{2.95} O ₁₆ | 16m | 87 | Ammonium cadmium bromide, (NH ₄) ₄ CdBr ₆ | 15m | 9 |
| Aluminum iron oxide, AlFeO ₃ | 15m | 7 | Ammonium cadmium chloride, NH ₄ CdCl ₃ | 5m | 6 |
| Aluminum lithium, Al ₄ Li ₉ | 10m | 98 | Ammonium cadmium sulfate, (NH ₄) ₂ Cd ₂ (SO ₄) ₃ | 7m | 5 |
| Aluminum nickel, AlNi | 6m | 82 | Ammonium cadmium sulfate hydrate, (NH ₄) ₂ Cd(SO ₄) ₂ ·6H ₂ O | 8m | 5 |
| Aluminum nitride, AlN | 12m | 5 | Ammonium calcium sulfate, (NH ₄) ₂ Ca ₂ (SO ₄) ₃ | 8m | 7 |
| Aluminum nitrate hydrate, Al(NO ₃) ₃ ·9H ₂ O | 11m | 6 | Ammonium chlorate, NH ₄ ClO ₄ (orthorhombic) | 7 | 6 |
| Aluminum oxide (corundum), α-Al ₂ O ₃ | 9 | 3 | Ammonium chloride (salammoniac), NH ₄ Cl | 1 | 59 |
| Aluminum oxide hydrate (boehmite), α-Al ₂ O ₃ ·H ₂ O | 3 | 38 | Ammonium chromium sulfate hydrate, NH ₄ Cr(SO ₄) ₂ ·12H ₂ O | 6 | 7 |
| Aluminum oxide hydrate, diaspore, β-Al ₂ O ₃ ·H ₂ O | 3 | 41 | Ammonium cobalt (II) chloride, NH ₄ CoCl ₃ | 6m | 5 |
| Aluminum phosphate, Al(PO ₃) ₃ | 2m | 3 | Ammonium cobalt fluoride, NH ₄ CoF ₃ | 8m | 9 |
| Aluminum phosphate (berlinite), AlPO ₄ (trigonal) | 10 | 3 | Ammonium copper bromide hydrate, (NH ₄) ₂ CuBr ₄ ·2H ₂ O | 10m | 6 |
| Aluminum phosphate, AlPO ₄ (orthorhombic) | 10 | 4 | Ammonium copper chloride, NH ₄ CuCl ₃ | 7m | 7 |
| Aluminum plutonium, Al ₃ Pu | 15m | 77 | Ammonium copper chloride hydrate, (NH ₄) ₂ CuCl ₄ ·2H ₂ O | 12m | 6 |
| Aluminum rhenium, AlRe | 15m | 79 | Ammonium copper fluoride, NH ₄ CuF ₃ | 11m | 8 |
| Aluminum rhenium, Al ₁₂ Re | 15m | 80 | Ammonium gallium sulfate hydrate, NH ₄ Ga(SO ₄) ₂ ·12H ₂ O | 6 | 9 |
| Aluminum rhodium, AlRh | 15m | 82 | Ammonium germanium fluoride, (NH ₄) ₂ GeF ₆ | 6 | 8 |
| Aluminum ruthenium, AlRu | 15m | 83 | Ammonium hydrogen arsenate, NH ₄ H ₂ AsO ₄ | 16m | 9 |
| Aluminum ruthenium, Al ₆ Ru | 15m | 84 | Ammonium hydrogen carbonate (teschemacherite), (NH ₄)HCO ₃ | 9 | 5 |
| Aluminum samarium, AlSm ₂ | 15m | 86 | Ammonium hydrogen phosphate, NH ₄ H ₂ PO ₄ | 4 | 64 |
| Aluminum samarium, AlSm ₃ | 15m | 88 | Ammonium iodate, NH ₄ IO ₃ | 10m | 7 |
| Aluminum samarium, Al ₂ Sm | 15m | 90 | Ammonium iodide, NH ₄ I | 4 | 56 |
| Aluminum samarium, Al ₃ Sm | 15m | 91 | Ammonium iridium chloride, (NH ₄) ₂ IrCl ₆ | 8 | 6 |
| Aluminum silicate (mullite), Al ₆ Si ₂ O ₁₃ | 3m | 3 | Ammonium iron chloride hydrate, (NH ₄) ₂ FeCl ₅ ·H ₂ O | 14m | 7 |
| Aluminum sulfate, Al ₂ (SO ₄) ₃ | 15m | 8 | Ammonium iron fluoride, (NH ₄) ₃ FeF ₆ | 9m | 9 |
| Aluminum technetium, Al ₆ Tc | 15m | 93 | Ammonium iron sulfate, NH ₄ Fe(SO ₄) ₂ | 10m | 8 |
| Aluminum terbium, Al ₂ Tb | 15m | 95 | Ammonium iron sulfate hydrate, NH ₄ Fe(SO ₄) ₂ ·12H ₂ O | 6 | 10 |
| Aluminum terbium, Al ₂ Tb ₃ | 15m | 96 | Ammonium lead chloride, (NH ₄) ₂ PbCl ₆ | 11m | 10 |
| Aluminum thorium uranium, Al ₆ ThU .. | 15m | 98 | Ammonium magnesium aluminum fluoride, NH ₄ MgAlF ₆ | 10m | 9 |
| Aluminum tungsten, Al ₅ W, δ-phase .. | 15m | 100 | Ammonium magnesium chromium oxide hydrate, (NH ₄) ₂ Mg(CrO ₄) ₂ ·6H ₂ O | 8m | 10 |
| Aluminum tungsten oxide, Al ₂ (WO ₄) ₃ | 11m | 7 | Ammonium magnesium phosphate hydrate (struvite), NH ₄ MgPO ₄ ·6H ₂ O | 3m | 41 |
| Aluminum vanadium, Al ₁₀ V | 15m | 102 | Ammonium manganese chloride hydrate, (NH ₄) ₂ MnCl ₄ ·2H ₂ O | 11m | 11 |
| Aluminum vanadium, Al _{10.25} V | 15m | 104 | | | |
| Aluminum vanadium, Al ₂₃ V ₄ | 15m | 106 | | | |
| Aluminum vanadium, Al ₄₅ V ₇ , α'-phase | 15m | 108 | | | |
| Aluminum ytterbium, Al ₂ Yb | 15m | 111 | | | |
| Aluminum yttrium, Al ₃ Y | 15m | 112 | | | |
| Ammonium aluminum fluoride, (NH ₄) ₃ AlF ₆ | 9m | 5 | | | |

Further work on this program is in progress, and it is anticipated that additional sections will be issued. Therefore, the cumulative index here is not necessarily the concluding index for the project.

m - Monograph 25.

A mineral name in () indicates a synthetic sample.

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|---|-----------------|------|--|-----------------|------|
| Ammonium manganese(II) fluoride, NH ₄ MnF ₃ | 5m | 8 | Antimony gadolinium, GdSb..... | 4m | 42 |
| Ammonium manganese sulfate, (NH ₄) ₂ Mn ₂ (SO ₄) ₃ | 7m | 8 | Antimony gallium, GaSb..... | 6 | 30 |
| Ammonium manganese sulfate hydrate, (NH ₄) ₂ Mn(SO ₄) ₂ ·6H ₂ O | 8m | 12 | Antimony gold (aurostibite), AuSb ₂ | 7 | 18 |
| Ammonium mercury chloride, NH ₄ HgCl ₃ | 8m | 14 | Antimony indium, InSb..... | 4 | 73 |
| Ammonium molybdenum oxide phosphate hydrate, (NH ₄) ₃ (MoO ₃) ₁₂ PO ₄ ·4H ₂ O .. | 8 | 10 | Antimony(III) iodide, SbI ₃ | 6 | 16 |
| Ammonium nickel(II) chloride, NH ₄ NiCl ₃ | 6m | 6 | Antimony iron titanium oxide hydroxide, derbylite, SbFe ₄ Ti ₃ O ₁₃ (OH)..... | 16m | 89 |
| Ammonium nickel chromium oxide hydrate, (NH ₄) ₂ Ni(CrO ₄) ₂ ·6H ₂ O | 8m | 16 | Antimony lanthanum, LaSb..... | 4m | 42 |
| Ammonium nickel sulfate hydrate, (NH ₄) ₂ Ni(SO ₄) ₂ ·6H ₂ O | 17m | 9 | Antimony neodymium, NdSb..... | 4m | 43 |
| Ammonium nitrate (nitrammite), NH ₄ NO ₃ | 7 | 4 | Antimony(III) oxide (senarmontite), Sb ₂ O ₃ (cubic) | 3 | 31 |
| Ammonium osmium bromide, (NH ₄) ₂ OsBr ₆ | 3 | 71 | Antimony(III) oxide, valentinite, Sb ₂ O ₃ (orthorhombic) | 10 | 6 |
| Ammonium osmium chloride, (NH ₄) ₂ OsCl ₆ | 1m | 6 | Antimony(IV) oxide (cervantite), Sb ₂ O ₄ | 10 | 8 |
| Ammonium palladium chloride, (NH ₄) ₂ PdCl ₄ | 6 | 6 | Antimony(V) oxide, Sb ₂ O ₅ | 10 | 10 |
| Ammonium palladium chloride, (NH ₄) ₂ PdCl ₆ | 8 | 7 | Antimony oxide, Sb ₆ O ₁₃ | 16m | 14 |
| Ammonium platinum bromide, (NH ₄) ₂ PtBr ₆ | 9 | 6 | Antimony praseodymium, PrSb..... | 4m | 43 |
| Ammonium platinum chloride, (NH ₄) ₂ PtCl ₆ | 5 | 3 | Antimony scandium, SbSc..... | 4m | 44 |
| Ammonium potassium iron chloride hydrate (kremersite), (NH ₄ ,K) ₂ FeCl ₅ ·H ₂ O | 14m | 8 | Antimony selenide, Sb ₂ Se ₃ | 3m | 7 |
| Ammonium rhenium oxide, NH ₄ ReO ₄ ... | 9 | 7 | Antimony silver sulfide, AgSbS ₂ (cubic)..... | 5m | 48 |
| Ammonium selenium bromide, (NH ₄) ₂ SeBr ₆ | 8 | 4 | Antimony silver sulfide (miargyrite), AgSbS ₂ (monoclinic)..... | 5m | 49 |
| Ammonium silicon fluoride (cryptohalite), (NH ₄) ₂ SiF ₆ | 5 | 5 | Antimony silver sulfide (pyrargyrite), Ag ₃ SbS ₃ (trigonal)..... | 5m | 51 |
| Ammonium strontium chromium oxide, (NH ₄) ₂ Sr(CrO ₄) ₂ | 14m | 9 | Antimony silver telluride, AgSbTe ₂ . | 3m | 47 |
| Ammonium strontium sulfate, (NH ₄) ₂ Sr(SO ₄) ₂ | 15m | 11 | Antimony(III) sulfide (stibnite), Sb ₂ S ₃ | 5 | 6 |
| Ammonium sulfate (mascagnite), (NH ₄) ₂ SO ₄ | 9 | 8 | Antimony telluride, Sb ₂ Te ₃ | 3m | 8 |
| Ammonium sulfate, (NH ₄) ₂ S ₂ O ₃ | 17m | 11 | Antimony terbium, SbTb..... | 5m | 61 |
| Ammonium sulfate, (NH ₄) ₂ S ₂ O ₈ | 17m | 13 | Antimony thorium, SbTh..... | 4m | 44 |
| Ammonium tellurium bromide, (NH ₄) ₂ TeBr ₆ | 8 | 5 | Antimony thulium, SbTm..... | 4m | 45 |
| Ammonium tellurium chloride, (NH ₄) ₂ TeCl ₆ | 8 | 8 | Antimony tin, SbSn..... | 16m | 15 |
| Ammonium tin chloride, (NH ₄) ₂ SnCl ₆ | 5 | 4 | Antimony ytterbium, SbYb..... | 4m | 45 |
| Ammonium titanium fluoride, (NH ₄) ₂ TiF ₆ | 16m | 10 | Antimony yttrium, SbY..... | 4m | 46 |
| Ammonium vanadium oxide, NH ₄ VO ₃ .. | 8 | 9 | Arsenic, As | 3 | 6 |
| Ammonium zinc chloride, (NH ₄) ₃ ZnCl ₅ | 15m | 12 | Arsenic cerium, AsCe..... | 4m | 51 |
| Ammonium zinc fluoride, NH ₄ ZnF ₃ ... | 8m | 18 | Arsenic(III) iodide, AsI ₃ | 13m | 7 |
| Ammonium zirconium fluoride, (NH ₄) ₃ ZrF ₇ | 6 | 14 | Arsenic oxide (arsenolite), As ₂ O ₃ (cubic) | 1 | 51 |
| Antimonic acid, H ₁₄ Sb ₁₄ O ₂₁ (OH) ₄₂ ... | 16m | 13 | Arsenic oxide, claudetite, As ₂ O ₃ (monoclinic) | 3m | 9 |
| Antimony, Sb | 3 | 14 | Barium, Ba | 4 | 7 |
| Antimony bromide, α-SbBr ₃ | 15m | 13 | Barium aluminum oxide, BaAl ₂ O ₄ | 5m | 11 |
| Antimony cerium, CeSb..... | 4m | 40 | Barium aluminum oxide, Ba ₃ Al ₂ O ₆ ... | 12m | 7 |
| Antimony cobalt, CoSb..... | 15m | 121 | Barium arsenate, Ba ₃ (AsO ₄) ₂ | 2m | 6 |
| Antimony cobalt, CoSb ₂ | 15m | 122 | Barium borate, BaB ₄ O ₇ | 4m | 6 |
| Antimony cobalt titanium, CoSbTi... | 15m | 124 | Barium borate, high form, BaB ₂ O ₄ .. | 4m | 4 |
| Antimony cobalt vanadium, CoSbV.... | 15m | 125 | Barium borate, BaB ₈ O ₁₃ | 7m | 10 |
| Antimony dysprosium, DySb..... | 4m | 41 | Barium bromate hydrate, Ba(BrO ₃) ₂ ·H ₂ O | 8m | 19 |
| Antimony erbium, ErSb..... | 4m | 41 | Barium bromide, BaBr ₂ | 10m | 63 |
| Antimony(III) fluoride, SbF ₃ | 2m | 4 | Barium bromide fluoride, BaBrF | 10m | 10 |
| | | | Barium bromide hydrate, BaBr ₂ ·H ₂ O | 3m | 10 |
| | | | Barium bromide hydrate, BaBr ₂ ·2H ₂ O | 16m | 16 |
| | | | Barium cadmium chloride hydrate, BaCdCl ₄ ·4H ₂ O..... | 15m | 14 |
| | | | Barium calcium nitrate, Ba _{2.25} Ca _{7.75} (NO ₃) ₂ | 12m | 38 |
| | | | Barium calcium nitrate, Ba ₅₀ Ca ₅₀ (NO ₃) ₂ | 12m | 38 |
| | | | Barium calcium nitrate, Ba ₇₅ Ca ₂₅ (NO ₃) ₂ | 12m | 38 |
| | | | Barium calcium tungsten oxide, Ba ₂ CaWO ₆ | 9m | 10 |

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| Barium carbonate (witherite), BaCO ₃ (orthorhombic) | 2 | 54 | Beryllium aluminum oxide (chrysoberyl), BeAl ₂ O ₄ | 9 | 10 |
| Barium carbonate, BaCO ₃ (cubic) at 1075 °C | 10 | 11 | Beryllium aluminum silicate, beryl, Be ₃ Al ₂ (SiO ₃) ₆ | 9 | 13 |
| Barium chlorate, Ba(ClO ₃) ₂ | 16m | 17 | Beryllium calcium iron magnesium aluminum phosphate hydroxide hydrate, roscherite (monoclinic), Be ₂ Ca(Fe ₃ Mg ₇) ₂ Al ₆₇ (PO ₄) ₃ (OH) ₃ ·2H ₂ O | 16m | 96 |
| Barium chlorate hydrate, Ba(ClO ₄) ₂ ·3H ₂ O | 2m | 7 | Beryllium calcium manganese aluminum iron phosphate hydroxide hydrate, roscherite (triclinic), Be ₄ Ca ₂ (Mn _{3.91} Mg _{0.04} Ca _{0.05})(Al ₁₃ Fe _{0.42} Mn ₁₂)(PO ₄) ₆ (OH) ₄ ·6H ₂ O | 16m | 100 |
| Barium chlorate hydrate, Ba(ClO ₃) ₂ ·H ₂ O | 8m | 21 | Beryllium calcium oxide, Be ₁₇ Ca ₁₂ O ₂₉ | 7m | 89 |
| Barium chloride, BaCl ₂ , (cubic) ... | 9m | 13 | Beryllium chromium oxide, BeCr ₂ O ₄ | 10 | 12 |
| Barium chloride, BaCl ₂ , (orthorhombic) | 9m | 11 | Beryllium cobalt, BeCo | 5m | 62 |
| Barium chloride fluoride, BaClF ... | 10m | 11 | Beryllium germanium oxide, Be ₂ GeO ₄ | 10 | 13 |
| Barium chloride hydrate, BaCl ₂ ·2H ₂ O | 12m | 9 | Beryllium lanthanum oxide, Be ₂ La ₂ O ₅ | 9m | 65 |
| Barium chromium oxide, Ba ₃ (CrO ₄) ₂ | 15m | 16 | Beryllium niobium, Be ₂ Nb | 7m | 92 |
| Barium fluoride, BaF ₂ | 1 | 70 | Beryllium oxide (bromellite), BeO | 1 | 36 |
| Barium hydroxide phosphate, Ba ₅ (OH)(PO ₄) ₃ | 11m | 12 | Beryllium palladium, BePd | 5m | 62 |
| Barium iodide, BaI ₂ | 10m | 66 | Beryllium silicate, phenakite, Be ₂ SiO ₄ | 8 | 11 |
| Barium iodide hydrate, BaI ₂ ·2H ₂ O ... | 16m | 18 | Beryllium sulfate, BeSO ₄ | 15m | 20 |
| Barium lead chloride, BaPbCl ₄ | 11m | 13 | Bismuth, Bi | 3 | 20 |
| Barium lead nitrate, Ba ₃₃ Pb ₆₇ (NO ₃) ₂ | 12m | 40 | Bismuth bromide oxide, BiOBr | 8 | 14 |
| Barium lead nitrate, Ba ₆₇ Pb ₃₃ (NO ₃) ₂ | 12m | 40 | Bismuth cerium, BiCe | 4m | 46 |
| Barium manganese oxide, Ba(MnO ₄) ₂ | 15m | 17 | Bismuth chloride oxide (bismoclite), BiOCl | 4 | 54 |
| Barium molybdenum oxide, BaMoO ₄ ... | 7 | 7 | Bismuth dysprosium, BiDy | 4m | 47 |
| Barium molybdenum oxide, Ba ₂ MoO ₅ .. | 12m | 10 | Bismuth erbium, BiEr | 4m | 47 |
| Barium nitrate (nitrobarite), Ba(NO ₃) ₂ | 11m | 14 | Bismuth fluoride, BiF ₃ | 1m | 7 |
| Barium nitrite hydrate, Ba(NO ₂) ₂ ·H ₂ O | 15m | 18 | Bismuth holmium, BiHo | 4m | 48 |
| Barium oxide, BaO | 9m | 63 | Bismuth(III) iodide, BiI ₃ | 6 | 20 |
| Barium oxide, BaO ₂ | 6 | 18 | Bismuth iodide oxide, BiOI | 9 | 16 |
| Barium phosphate, Ba ₂ P ₂ O ₇ , (high form) | 16m | 19 | Bismuth lanthanum, BiLa | 4m | 48 |
| Barium phosphate, Ba ₃ (PO ₄) ₂ | 12m | 12 | Bismuth neodymium, BiNd | 4m | 49 |
| Barium selenide, BaSe | 5m | 61 | Bismuth oxide (bismite), α-Bi ₂ O ₃ .. | 3m | 16 |
| Barium silicate, β-BaSiO ₃ | 13m | 8 | Bismuth phosphate, BiPO ₄ (monoclinic) | 3m | 11 |
| Barium silicate (sanbornite), β-BaSi ₂ O ₅ | 13m | 10 | Bismuth phosphate, BiPO ₄ (trigonal) | 3m | 13 |
| Barium silicate, Ba ₂ SiO ₄ | 13m | 12 | Bismuth praseodymium, BiPr | 4m | 49 |
| Barium silicate, Ba ₂ Si ₃ O ₈ | 13m | 13 | Bismuth sulfide (bismuthinite), Bi ₂ S ₃ | 5m | 13 |
| Barium silicate, Ba ₃ SiO ₅ | 13m | 15 | Bismuth telluride, BiTe | 4m | 50 |
| Barium silicate, Ba ₃ Si ₅ O ₁₃ | 13m | 17 | Bismuth telluride (tellurobis- muthite), Bi ₂ Te ₃ | 3m | 16 |
| Barium silicon fluoride, BaSiF ₆ ... | 4m | 7 | Bismuth vanadium oxide, low form, BiVO ₄ (tetragonal) | 3m | 14 |
| Barium strontium nitrate, Ba ₂₅ Sr ₇₅ (NO ₃) ₂ | 12m | 42 | Bismuth vanadium oxide, high form, BiVO ₄ (monoclinic) | 3m | 14 |
| Barium strontium nitrate, Ba ₅₀ Sr ₅₀ (NO ₃) ₂ | 12m | 42 | Boron oxide, B ₂ O ₃ , phase 1 | 10m | 70 |
| Barium strontium nitrate, Ba ₇₅ Sr ₂₅ (NO ₃) ₂ | 12m | 42 | Cadmium, Cd | 3 | 10 |
| Barium sulfate (baryte), BaSO ₄ | 10m | 12 | Cadmium ammine chloride, Cd(NH ₃) ₂ Cl ₂ | 10m | 14 |
| Barium sulfide, BaS | 7 | 8 | Cadmium borate, CdB ₄ O ₇ | 16m | 24 |
| Barium thiosulfate hydrate, BaS ₂ O ₃ ·H ₂ O | 16m | 20 | Cadmium bromate hydrate, Cd(BrO ₃) ₂ ·2H ₂ O | 17m | 14 |
| Barium tin oxide, BaSnO ₃ | 3m | 11 | Cadmium bromide, CdBr ₂ | 9 | 17 |
| Barium titanium oxide, BaTiO ₃ | 3 | 45 | Cadmium bromide chloride, CdBrCl .. | 11m | 15 |
| Barium titanium silicate (fresnoite), Ba ₂ TiSi ₂ O ₈ | 9m | 14 | Cadmium carbonate (otavite), CdCO ₃ .. | 7 | 11 |
| Barium tungsten oxide, BaWO ₄ | 7 | 9 | Cadmium cerium, CdCe | 5m | 63 |
| Barium tungsten oxide, Ba ₂ WO ₅ | 12m | 14 | Cadmium chlorate hydrate, Cd(ClO ₄) ₂ ·6H ₂ O | 3m | 19 |
| Barium vanadium oxide, Ba ₃ (VO ₄) ₂ .. | 14m | 10 | Cadmium chloride, CdCl ₂ | 9 | 18 |
| Barium zirconium oxide, BaZrO ₃ | 5 | 8 | Cadmium chromium oxide, CdCr ₂ O ₄ ... | 5m | 16 |
| Beryllium, alpha, Be | 9m | 64 | | | |

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| Cadmium copper, Cd_8Cu_5 | 11m | 81 | Calcium chromium silicate (uvarovite), $\text{Ca}_3\text{Cr}_2(\text{SiO}_4)_3$ | 10 | 17 |
| Cadmium cyanide, $\text{Cd}(\text{CN})_2$ | 2m | 8 | Calcium fluoride (fluorite), CaF_2 .. | 1 | 69 |
| Cadmium fluoride, CdF_2 | 10m | 15 | Calcium fluoride phosphate (fluorapatite), $\text{Ca}_5\text{F}(\text{PO}_4)_3$ | 3m | 22 |
| Cadmium iron oxide, CdFe_2O_4 | 9m | 16 | Calcium fluoride phosphate hydrate, $\text{CaFPO}_3 \cdot 2\text{H}_2\text{O}$ | 15m | 24 |
| Cadmium lanthanum, CdLa | 5m | 63 | Calcium gallium germanium oxide, $\text{Ca}_3\text{Ga}_2(\text{GeO}_4)_3$ | 10 | 18 |
| Cadmium manganese oxide, CdMn_2O_4 .. | 10m | 16 | Calcium hydrogen phosphate hydrate, $\text{Ca}_8\text{H}_2(\text{PO}_4)_6 \cdot 5\text{H}_2\text{O}$ | 13m | 21 |
| Cadmium molybdenum oxide, CdMoO_4 .. | 6 | 21 | Calcium hydrogen phosphate sulfate hydrate, $\text{Ca}_2\text{HPO}_4\text{SO}_4 \cdot 4\text{H}_2\text{O}$ | 16m | 109 |
| Cadmium nitrate hydrate, $\text{Cd}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$ | 7m | 93 | Calcium hydroxide (portlandite), $\text{Ca}(\text{OH})_2$ | 1 | 58 |
| Cadmium oxide, CdO | 2 | 27 | Calcium iodate (lautarite), $\text{Ca}(\text{IO}_3)_2$ | 14m | 12 |
| Cadmium oxide, CdO (ref. standard) | 8m | 2 | Calcium iodate hydrate, $\text{Ca}(\text{IO}_3)_2 \cdot 6\text{H}_2\text{O}$ | 14m | 13 |
| Cadmium phosphate, $\text{Cd}_2\text{P}_2\text{O}_7$ | 16m | 26 | Calcium iron germanium oxide, $\text{Ca}_3\text{Fe}_2(\text{GeO}_4)_3$ | 10 | 19 |
| Cadmium phosphate, $\text{Cd}_3(\text{PO}_4)_2$ | 16m | 27 | Calcium iron silicate (andradite), $\text{Ca}_3\text{Fe}_2\text{Si}_3\text{O}_{12}$ | 9 | 22 |
| Cadmium praseodymium, CdPr | 5m | 64 | Calcium iron silicate hydroxide, julgoldite, $\text{Ca}_2\text{Fe}_3\text{Si}_3\text{O}_{10}(\text{OH},\text{O})_2(\text{OH})_2$ | 10m | 72 |
| Cadmium selenide (cadmoselite), CdSe (hexagonal) | 7 | 12 | Calcium lead nitrate, $\text{Ca}_{.33}\text{Pb}_{.67}(\text{NO}_3)_2$ | 12m | 44 |
| Cadmium silicate, Cd_2SiO_4 | 13m | 19 | Calcium lead nitrate, $\text{Ca}_{.67}\text{Pb}_{.33}(\text{NO}_3)_2$ | 12m | 44 |
| Cadmium silicate, Cd_3SiO_5 | 13m | 20 | Calcium magnesium silicate (diopside), $\text{CaMg}(\text{SiO}_3)_2$ | 5m | 17 |
| Cadmium sulfate, CdSO_4 | 3m | 20 | Calcium molybdenum oxide (powellite), CaMoO_4 | 6 | 22 |
| Cadmium sulfate hydrate, $3\text{CdSO}_4 \cdot 8\text{H}_2\text{O}$ | 6m | 8 | Calcium nitrate, $\text{Ca}(\text{NO}_3)_2$ | 7 | 14 |
| Cadmium sulfate hydrate, $\text{CdSO}_4 \cdot \text{H}_2\text{O}$ | 6m | 10 | Calcium oxide (lime), CaO | 1 | 43 |
| Cadmium sulfide (greenockite), CdS | 4 | 15 | Calcium oxide (lime), CaO (calculated pattern) | 14m | 49 |
| Cadmium telluride, CdTe | 3m | 21 | Calcium oxide phosphate, $\text{Ca}_4\text{O}(\text{PO}_4)_2$ | 12m | 17 |
| Cadmium titanium oxide, CdTiO_3 | 15m | 21 | Calcium phosphate, $\beta\text{-Ca}_2\text{P}_2\text{O}_7$ | 7m | 95 |
| Cadmium tungsten oxide, CdWO_4 | 2m | 8 | Calcium platinum oxide, Ca_4PtO_6 ... | 10m | 18 |
| Calcium, Ca | 9m | 68 | Calcium selenide, CaSe | 5m | 64 |
| Calcium aluminum germanium oxide, $\text{Ca}_3\text{Al}_2(\text{GeO}_4)_3$ | 10 | 15 | Calcium strontium nitrate, $\text{Ca}_{.33}\text{Sr}_{.67}(\text{NO}_3)_2$ | 12m | 46 |
| Calcium aluminum hydroxide, $\text{Ca}_3\text{Al}_2(\text{OH})_{12}$ | 11m | 16 | Calcium strontium nitrate, $\text{Ca}_{.67}\text{Sr}_{.33}(\text{NO}_3)_2$ | 12m | 46 |
| Calcium aluminum iron oxide (brownmillerite), $\text{Ca}_4\text{Al}_2\text{Fe}_2\text{O}_{10}$ | 16m | 28 | Calcium sulfate (anhydrite), CaSO_4 | 4 | 65 |
| Calcium aluminum oxide, $\text{Ca}_3\text{Al}_2\text{O}_6$.. | 5 | 10 | Calcium sulfate hydrate (gypsum), $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$ | 17m | 16 |
| Calcium aluminum oxide (mayenite), $\text{Ca}_{12}\text{Al}_{14}\text{O}_{33}$ | 9 | 20 | Calcium sulfide (oldhamite), CaS .. | 7 | 15 |
| Calcium aluminum sulfate hydrate (ettringite), $\text{Ca}_6\text{Al}_2\text{S}_3\text{O}_{18} \cdot 3\text{H}_2\text{O}$.. | 8 | 3 | Calcium telluride, CaTe | 4m | 50 |
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| Calcium borate hydrate, hexahydroborite, $\text{Ca}[\text{B}(\text{OH})_4]_2 \cdot 2\text{H}_2\text{O}$ | 16m | 104 | Calcium titanium oxide (perovskite), CaTiO_3 | 9m | 17 |
| Calcium boride, CaB_6 | 16m | 29 | Calcium tungsten oxide, Ca_3WO_6 | 9m | 19 |
| Calcium bromide, CaBr_2 | 11m | 70 | Calcium tungsten oxide, scheelite, CaWO_4 | 6 | 23 |
| Calcium bromide hydrate, $\text{CaBr}_2 \cdot 6\text{H}_2\text{O}$ | 8 | 15 | Carbon, diamond, C | 2 | 5 |
| Calcium carbonate (aragonite), CaCO_3 (orthorhombic) | 3 | 53 | Cerium arsenate, CeAsO_4 | 4m | 8 |
| Calcium carbonate (aragonite), CaCO_3 (orthorhombic, calculated pattern) | 14m | 44 | Cerium(III) chloride, CeCl_3 | 1m | 8 |
| Calcium carbonate (calcite), CaCO_3 (hexagonal) | 2 | 51 | Cerium cobalt, CeCo_2 | 13m | 50 |
| Calcium chloride (hydrophilite), CaCl_2 | 11m | 18 | Cerium cobalt, $\text{Ce}_{24}\text{Co}_{11}$ | 13m | 51 |
| Calcium chloride fluoride, CaClF .. | 10m | 17 | Cerium copper, CeCu_6 | 7m | 99 |
| Calcium chloride hydrate, $\text{CaCl}_2 \cdot 4\text{H}_2\text{O}$ | 11m | 73 | Cerium(III) fluoride, CeF_3 | 8 | 17 |
| Calcium chloride hydrate (antarcticite), $\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$ | 12m | 16 | Cerium gallium, CeGa_2 | 13m | 54 |
| Calcium chromium germanium oxide, $\text{Ca}_3\text{Cr}_2(\text{GeO}_4)_3$ | 10 | 16 | Cerium magnesium, CeMg | 5m | 65 |
| Calcium chromium iron titanium oxide, loweringite, $\text{Ca}_{.72}\text{RE}_{.33}(\text{Y},$ $\text{Th}, \text{U}, \text{Pb})_{.05}\text{Ti}_{12.48}\text{Fe}_{3.38}\text{Cr}_{2.24}$ $\text{Mg}_{.92}\text{Zr}_{.58}\text{Al}_{.39}\text{V}_{.21}\text{Mn}_{.04}\text{O}_{38}$ | 16m | 106 | Cerium magnesium, CeMg_3 | 13m | 56 |
| Calcium chromium oxide (chromatite), CaCrO_4 | 7 | 13 | | | |
| Calcium chromium oxide, $\text{Ca}_3(\text{CrO}_4)_2$ | 15m | 22 | | | |

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| Cerium nickel, CeNi_2 | 13m | 58 | Cesium magnesium chromium oxide hydrate, $\text{Cs}_2\text{Mg}(\text{CrO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 8m | 29 |
| Cerium niobium titanium oxide (aeschnite), CeNbTiO_6 | 3m | 24 | Cesium magnesium sulfate hydrate, $\text{Cs}_2\text{Mg}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 7m | 18 |
| Cerium nitrate hydrate, $\text{Ce}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ | 17m | 20 | Cesium manganese fluoride, CsMnF_3 | 10m | 21 |
| Cerium nitride, CeN | 4m | 51 | Cesium manganese sulfate hydrate, $\text{Cs}_2\text{Mn}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 7m | 20 |
| Cerium(IV) oxide (cerianite), CeO_2 | 1 | 56 | Cesium mercury chloride, CsHgCl_3 .. | 7m | 22 |
| Cerium phosphide, CeP | 4m | 52 | Cesium nickel(II) chloride, CsNiCl_3 .. | 6m | 12 |
| Cerium thallium, CeTl | 13m | 59 | Cesium nickel sulfate hydrate, $\text{Cs}_2\text{Ni}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 7m | 23 |
| Cerium thallium, Ce_3Tl | 13m | 60 | Cesium nitrate, CsNO_3 | 9 | 25 |
| Cerium thallium, Ce_3Tl | 13m | 61 | Cesium osmium(IV) bromide, Cs_2OsBr_6 .. | 2m | 10 |
| Cerium(III) vanadium oxide, CeVO_4 .. | 1m | 9 | Cesium osmium chloride, Cs_2OsCl_6 .. | 2m | 11 |
| Cerium zinc, CeZn | 5m | 65 | Cesium platinum bromide, Cs_2PtBr_6 .. | 8 | 19 |
| Cerium zinc, CeZn_3 | 14m | 50 | Cesium platinum chloride, Cs_2PtCl_6 .. | 5 | 14 |
| Cerium zinc, CeZn_5 | 14m | 53 | Cesium platinum fluoride, Cs_2PtF_6 .. | 6 | 27 |
| Cerium zinc, $\text{Ce}_2\text{Zn}_{17}$ | 14m | 55 | Cesium selenium bromide, Cs_2SeBr_6 .. | 8 | 20 |
| Cesium aluminum sulfate hydrate, $\text{CsAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 6 | 25 | Cesium silicon fluoride, Cs_2SiF_6 .. | 5 | 19 |
| Cesium antimony fluoride, CsSbF_6 .. | 4m | 9 | Cesium strontium chloride, CsSrCl_3 .. | 6m | 13 |
| Cesium beryllium fluoride, CsBeF_3 .. | 9m | 69 | Cesium sulfate, Cs_2SO_4 | 7 | 17 |
| Cesium boron fluoride, CsBF_4 | 8 | 22 | Cesium tellurium bromide, Cs_2TeBr_6 .. | 9 | 24 |
| Cesium bromate, CsBrO_3 | 8 | 18 | Cesium tin chloride, Cs_2SnCl_6 | 5 | 16 |
| Cesium bromide, CsBr | 3 | 49 | Cesium vanadium sulfate hydrate, $\text{CsV}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 1m | 11 |
| Cesium cadmium bromide, CsCdBr_3 (hexagonal) | 10m | 20 | Cesium zinc sulfate hydrate, $\text{Cs}_2\text{Zn}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 7m | 25 |
| Cesium cadmium chloride, CsCdCl_3 (hexagonal) | 5m | 19 | Chromium, Cr | 5 | 20 |
| Cesium calcium chloride, CsCaCl_3 .. | 5m | 21 | Chromium boride, $\zeta\text{-CrB}$ | 17m | 22 |
| Cesium calcium fluoride, CsCaF_3 | 8m | 25 | Chromium chloride, CrCl_2 | 11m | 77 |
| Cesium calcium sulfate, $\text{Cs}_2\text{Ca}_2(\text{SO}_4)_3$ | 7m | 12 | Chromium chloride, CrCl_3 | 17m | 23 |
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| Cesium chlorate, CsClO_4 , (orthorhombic) | 1m | 10 | Chromium cobalt silicide, $\text{Co}_9\text{Cr}_{15}\text{Si}_6$ | 14m | 62 |
| Cesium chloride, CsCl | 2 | 44 | Chromium cobalt tantalum, CoCrTa .. | 15m | 142 |
| Cesium chromium oxide, Cs_2CrO_4 | 3m | 25 | Chromium fluoride, CrF_2 | 10m | 81 |
| Cesium chromium sulfate hydrate, $\text{CsCr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 8 | 21 | Chromium fluoride, Cr_2F_5 | 7m | 108 |
| Cesium cobalt(II) chloride, CsCoCl_3 .. | 6m | 11 | Chromium(III) fluoride hydrate, $\text{CrF}_3 \cdot 3\text{H}_2\text{O}$ | 5m | 25 |
| Cesium cobalt chloride, Cs_2CoCl_4 .. | 11m | 19 | Chromium iridium, Cr_3Ir | 6m | 14 |
| Cesium copper(II) chloride, CsCuCl_3 .. | 5m | 22 | Chromium iron oxide, $\text{Cr}_{1.3}\text{Fe}_{0.7}\text{O}_3$ | 17m | 24 |
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| Cesium copper sulfate hydrate, $\text{Cs}_2\text{Cu}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 7m | 14 | Chromium(III) oxide, Cr_2O_3 | 5 | 22 |
| Cesium fluoride, CsF | 3m | 26 | Chromium phosphate, $\alpha\text{-CrPO}_4$ | 2m | 12 |
| Cesium gallium sulfate hydrate, $\text{CsGa}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 8 | 23 | Chromium phosphate, $\beta\text{-CrPO}_4$ | 9 | 26 |
| Cesium germanium fluoride, Cs_2GeF_6 .. | 5 | 17 | Chromium phosphate hydrate, $\text{CrPO}_4 \cdot 6\text{H}_2\text{O}$ | 15m | 27 |
| Cesium iodate, CsIO_3 | 15m | 26 | Chromium rhodium, Cr_3Rh | 6m | 15 |
| Cesium iodide, CsI | 4 | 47 | Chromium silicide, Cr_3Si | 6 | 29 |
| Cesium iodine bromide, CsI_2Br | 7m | 103 | Chromium sulfate, $\text{Cr}_2(\text{SO}_4)_3$ | 16m | 33 |
| Cesium iodine chloride, CsI_2Cl_2 | 3 | 50 | Cobalt, Co (cubic) | 4m | 10 |
| Cesium iron chloride hydrate, $\text{Cs}_2\text{FeCl}_5 \cdot \text{H}_2\text{O}$ | 14m | 14 | Cobalt aluminum oxide, CoAl_2O_4 | 9 | 27 |
| Cesium iron sulfate hydrate, $\text{Cs}_2\text{Fe}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 7m | 16 | Cobalt ammine iodide, $\text{Co}(\text{NH}_3)_6\text{I}_3$.. | 10m | 83 |
| Cesium iron sulfate hydrate, $\text{CsFe}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 6 | 28 | Cobalt antimony oxide, CoSb_2O_6 | 5m | 26 |
| Cesium lead(II) chloride, CsPbCl_3 (tetragonal) | 5m | 24 | Cobalt arsenide, CoAs_2 | 4m | 10 |
| Cesium lead fluoride, CsPbF_3 | 8m | 26 | Cobalt arsenide (skutterudite), CoAs_3 | 10 | 21 |
| Cesium lithium cobalt cyanide, $\text{CsLiCo}(\text{CN})_6$ | 10m | 79 | Cobalt borate, $\text{Co}_3(\text{BO}_3)_2$ | 12m | 20 |
| Cesium lithium fluoride, CsLiF_2 ... | 7m | 105 | Cobalt bromide hydrate, $\text{CoBr}_2 \cdot 6\text{H}_2\text{O}$.. | 12m | 21 |
| Cesium magnesium chromium oxide, $\text{Cs}_2\text{Mg}_2(\text{CrO}_4)_3$ | 8m | 27 | Cobalt(II) carbonate (sphaero- cobaltite), CoCO_3 | 10 | 24 |
| | | | Cobalt chlorate hydrate, $\text{Co}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 3m | 28 |
| | | | Cobalt chloride hydrate, $\text{CoCl}_2 \cdot 2\text{H}_2\text{O}$.. | 11m | 22 |
| | | | Cobalt chloride hydrate, $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$.. | 11m | 23 |

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| Cobalt copper tin, CoCu_2Sn | 14m | 64 | Cobalt(II,III) oxide, Co_3O_4 | 9 | 29 |
| Cobalt dysprosium, Co_2Dy | 13m | 63 | Cobalt phosphate, $\text{Co}(\text{PO}_3)_2$ | 13m | 23 |
| Cobalt erbium, Co_2Er | 13m | 64 | Cobalt phosphide, CoP | 14m | 83 |
| Cobalt erbium, Co_7Er_2 | 13m | 65 | Cobalt phosphide, CoP_3 | 14m | 85 |
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| Cobalt gadolinium, Co_2Gd | 13m | 71 | (disordered) | 15m | 169 |
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| Cobalt gallium manganese, Co_2GaMn | 13m | 75 | Cobalt plutonium, CoPu_3 | 15m | 171 |
| Cobalt gallium niobium, | | | Cobalt plutonium, CoPu_6 | 14m | 89 |
| $\text{Co}_{1.5}\text{Ga}_{0.5}\text{Nb}$ | 15m | 144 | Cobalt plutonium, Co_2Pu | 14m | 91 |
| Cobalt gallium niobium, Co_2GaNb ... | 14m | 66 | Cobalt plutonium, Co_3Pu | 14m | 92 |
| Cobalt gallium oxide, CoGa_2O_4 | 10 | 27 | Cobalt plutonium, $\text{Co}_{17}\text{Pu}_2$ | 14m | 94 |
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| $\text{Co}_{1.5}\text{Ga}_{0.5}\text{Ta}$ | 15m | 146 | Cobalt rhodium sulfide, Co_8RhS_8 ... | 14m | 98 |
| Cobalt gallium tantalum, Co_2GaTa | 13m | 76 | Cobalt ruthenium sulfide, Co_8RuS_8 .. | 14m | 100 |
| Cobalt gallium titanium, Co_2GaTi .. | 13m | 77 | Cobalt samarium, Co_2Sm | 15m | 173 |
| Cobalt gallium vanadium, Co_2GaV ... | 13m | 78 | Cobalt samarium, Co_5Sm | 13m | 90 |
| Cobalt germanium, Co_3Ge_2 | 14m | 67 | Cobalt silicate, Co_2SiO_4 | | |
| Cobalt germanium, Co_5Ge_7 | 15m | 148 | (orthorhombic) | 4m | 11 |
| Cobalt germanium hafnium, | | | Cobalt silicon fluoride hydrate, | | |
| $\text{Co}_{16}\text{Ge}_7\text{Hf}_6$ | 14m | 69 | $\text{CoSiF}_6 \cdot 6\text{H}_2\text{O}$ | 3m | 27 |
| Cobalt germanium manganese, | | | Cobalt sulfate, $\beta\text{-CoSO}_4$ | 2m | 14 |
| Co_2GeMn | 13m | 79 | Cobalt tantalum silicide, | | |
| Cobalt germanium niobium, | | | $\text{Co}_{16}\text{Ta}_6\text{Si}_7$ | 14m | 102 |
| $\text{Co}_{1.5}\text{Ge}_{0.5}\text{Nb}$ | 15m | 150 | Cobalt thorium, $\text{Co}_{17}\text{Th}_2$ | 12m | 64 |
| Cobalt germanium niobium, | | | Cobalt tin, Co_3Sn_2 | 13m | 92 |
| $\text{Co}_{16}\text{Ge}_7\text{Nb}_6$ | 14m | 71 | Cobalt tin oxide, Co_2SnO_4 | 15m | 30 |
| Cobalt germanium oxide, Co_2GeO_4 ... | 10 | 27 | Cobalt tin vanadium, Co_2SnV | 15m | 174 |
| Cobalt germanium tantalum, | | | Cobalt tin zirconium, Co_2SnZr | 15m | 175 |
| $\text{Co}_{1.5}\text{Ge}_{0.5}\text{Ta}$ | 15m | 152 | Cobalt titanium oxide, CoTiO_3 | 4m | 13 |
| Cobalt germanium tantalum, | | | Cobalt titanium silicide, | | |
| $\text{Co}_{16}\text{Ge}_7\text{Ta}_6$ | 14m | 73 | $\text{Co}_{16}\text{Ti}_6\text{Si}_7$ | 14m | 104 |
| Cobalt germanium titanium, Co_2GeTi | 13m | 80 | Cobalt tungsten oxide, CoWO_4 | 4m | 13 |
| Cobalt hafnium tin, Co_2HfSn | 14m | 75 | Cobalt vanadium silicide, Co_2VSi .. | 15m | 176 |
| Cobalt holmium, Co_2Ho | 14m | 76 | Copper, Cu | 1 | 15 |
| Cobalt holmium, $\text{Co}_9\text{Ho}_{12}$ | 15m | 154 | Copper ammine selenate, | | |
| Cobalt hydroxide, $\beta\text{-Co}(\text{OH})_2$ | 15m | 29 | $\text{Cu}(\text{NH}_3)_4\text{SeO}_4$ | 10m | 87 |
| Cobalt indium, CoIn_3 | 13m | 81 | Copper ammine sulfate hydrate, | | |
| Cobalt iodide, CoI_2 | 4m | 52 | $\text{Cu}(\text{NH}_3)_4\text{SO}_4 \cdot \text{H}_2\text{O}$ | 10m | 90 |
| Cobalt iron arsenide | | | Copper antimony oxide, CuSb_2O_6 | 5m | 27 |
| (safflorite), CoFeAs_4 | 10 | 28 | Copper arsenate (trippkeite), | | |
| Cobalt iron oxide, CoFe_2O_4 | 9m | 22 | CuAs_2O_4 | 16m | 120 |
| Cobalt iron sulfide, Co_8FeS_8 | 14m | 77 | Copper(I) bromide, CuBr | 4 | 36 |
| Cobalt iron vanadium, | | | Copper(I) chloride (nantokite), | | |
| $\text{Co}_4\text{Fe}_{13}\text{V}_{12}\text{Si}_{18}$ | 14m | 79 | CuCl | 4 | 35 |
| Cobalt lanthanum, CoLa_3 | 13m | 83 | Copper fluoride hydrate, $\text{CuF}_2 \cdot 2\text{H}_2\text{O}$ | 11m | 25 |
| Cobalt lutetium, Co_2Lu | 13m | 86 | Copper hydrogen phosphite hydrate, | | |
| Cobalt magnesium, Co_2Mg | 15m | 156 | $\text{CuHPO}_3 \cdot 2\text{H}_2\text{O}$ | 11m | 83 |
| Cobalt manganese silicide, Co_2MnSi | 14m | 81 | Copper hydroxide carbonate, | | |
| Cobalt mercury thiocyanate, | | | azurite, $\text{Cu}_3(\text{OH})_2(\text{CO}_3)_2$ | 10 | 30 |
| $\text{Co}[\text{Hg}(\text{CNS})_4]$ | 2m | 13 | Copper hydroxide carbonate | | |
| Cobalt molybdenum, Co_2Mo | 14m | 82 | (malachite), $\text{Cu}_2(\text{OH})_2\text{CO}_3$ | 10 | 31 |
| Cobalt molybdenum, Co_2Mo_3 | 15m | 158 | Copper hydroxide phosphate | | |
| Cobalt molybdenum, Co_7Mo_6 | 15m | 160 | (libethenite), $\text{Cu}_2(\text{OH})\text{PO}_4$ | 17m | 30 |
| Cobalt molybdenum silicide, | | | Copper(I) iodide (marshite), CuI .. | 4 | 38 |
| $\text{Co}_3\text{Mo}_2\text{Si}$ | 15m | 162 | Copper lead hydroxide sulfate, | | |
| Cobalt neodymium, Co_2Nd | 13m | 87 | linarite, $\text{CuPb}(\text{OH})_2(\text{SO}_4)$ | 16m | 34 |
| Cobalt nickel tin, | | | Copper(I) oxide (cuprite), Cu_2O ... | 2 | 23 |
| $\text{Co}_{75}\text{Ni}_{75}\text{Sn}_{75}$ | 13m | 88 | Copper(II) oxide (tenorite), CuO .. | 1 | 49 |
| Cobalt niobium silicide, $\text{Co}_3\text{Nb}_4\text{Si}_7$ | 15m | 164 | Copper phosphate, $\text{Cu}(\text{PO}_3)_2$ | 14m | 15 |
| Cobalt niobium tin, Co_2NbSn | 15m | 166 | Copper phosphate, $\alpha\text{-Cu}_2\text{P}_2\text{O}_7$ | 7m | 113 |
| Cobalt nitrate hydrate, | | | Copper sulfate (chalcocyanite), | | |
| $\alpha\text{-Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ | 12m | 22 | CuSO_4 | 3m | 29 |

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| Copper uranium oxide, CuUO ₄ | 10m | 93 | (tetragonal) (high form) | 8 | 28 |
| Dichlorotetraaquo chromium (III) | | | Gold, Au | 1 | 33 |
| chloride dihydrate, [Cr(H ₂ O) ₄ Cl ₂] | | | Gold chloride, AuCl | 16m | 37 |
| Cl·2H ₂ O | 16m | 31 | Gold(I) cyanide, AuCN | 10 | 33 |
| Dysprosium arsenate, DyAsO ₄ | 3m | 30 | Gold holmium, AuHo | 5m | 68 |
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| Dysprosium gallium oxide, | | | Gold niobium, AuNb ₃ | 6m | 16 |
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| Dysprosium nitride, DyN | 4m | 53 | Gold titanium, AuTi ₃ | 6m | 17 |
| Dysprosium oxide, Dy ₂ O ₃ | 9 | 30 | Gold vanadium, AuV ₃ | 6m | 18 |
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| Erbium gallium oxide, Er ₃ Ga ₅ O ₁₂ ... | 1m | 12 | Holmium selenide, HoSe | 4m | 59 |
| Erbium manganese oxide, ErMnO ₃ | 2m | 16 | Holmium silver, HoAg | 5m | 68 |
| Erbium nitride, ErN | 4m | 55 | Holmium vanadium oxide, HoVO ₄ | 4m | 18 |
| Erbium oxide, Er ₂ O ₃ | 8 | 25 | Hydrazinium sulfate, (NH ₃) ₂ SO ₄ | 17m | 38 |
| Erbium phosphate, ErPO ₄ | 9 | 31 | Hydrogen amidosulfate, H ₂ NSO ₃ H | 7 | 54 |
| Erbium silver, ErAg | 5m | 67 | Hydrogen arsenate, H ₅ As ₃ O ₁₀ | 7m | 84 |
| Erbium telluride, ErTe | 4m | 55 | Hydrogen borate, β-HBO ₂ (monoclinic) | 9m | 71 |
| Erbium vanadium oxide, ErVO ₄ | 5m | 29 | Hydrogen borate (metaborite), | | |
| Europium arsenate, EuAsO ₄ | 3m | 32 | HBO ₂ (cubic) | 4m | 27 |
| Europium(III) chloride, EuCl ₃ | 1m | 13 | Hydrogen iodate, HIO ₃ | 5 | 28 |
| Europium chloride oxide, EuClO | 1m | 13 | Hydrogen iodate, HI ₃ O ₈ | 8m | 104 |
| Europium gallium oxide, | | | Hydrogen phosphate hydrate, | | |
| Eu ₃ Ga ₅ O ₁₂ | 2m | 17 | H ₃ PO ₄ ·0.5H ₂ O | 12m | 56 |
| Europium nitride, EuN | 4m | 56 | Hydrogen tellurate, H ₆ TeO ₆ | 12m | 34 |
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| Europium phosphate, EuPO ₄ | 11m | 26 | Indium arsenide, InAs | 3m | 35 |
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| Gadolinium arsenate, GdAsO ₄ | 4m | 17 | Indium phosphate, InPO ₄ | 8 | 29 |
| Gadolinium arsenide, GdAs | 4m | 57 | Indium sulfide, In ₂ S ₃ | 11m | 30 |
| Gadolinium chloride hydrate, | | | Iodine, I ₂ | 3 | 16 |
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| Gadolinium chloride oxide, GdClO .. | 1m | 17 | Iridium niobium, IrNb ₃ | 6m | 19 |
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| Gadolinium silver, GdAg | 6m | 87 | Iron bromide, FeBr ₂ | 4m | 59 |
| Gadolinium titanium oxide, Gd ₂ TiO ₅ | 8m | 32 | Iron carbonate, siderite, FeCO ₃ ... | 15m | 32 |
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| Gallium, Ga | 2 | 9 | Iron chloride hydrate (hydromolysite), | | |
| Gallium arsenide, GaAs | 3m | 33 | FeCl ₃ ·6H ₂ O | 17m | 40 |
| Gallium lutetium oxide, Ga ₅ Lu ₃ O ₁₂ | 2m | 22 | Iron fluoride hydrate, FeF ₂ ·4H ₂ O | 11m | 90 |
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| Gallium magnesium, Ga ₅ Mg ₂ | 12m | 51 | Iron hydroxide sulfate hydrate, | | |
| Gallium neodymium oxide, Ga ₅ Nd ₃ O ₁₂ | 1m | 34 | butlerite, Fe(OH)SO ₄ ·2H ₂ O | 10m | 95 |
| Gallium oxide, α-Ga ₂ O ₃ | 4 | 25 | Iron iodide, FeI ₂ | 4m | 60 |
| Gallium phosphate (α-quartz type), | | | Iron(II,III) oxide (magnetite), | | |
| GaPO ₄ | 8 | 27 | Fe ₃ O ₄ | 5m | 31 |
| Gallium phosphate hydrate, | | | Iron phosphate, FePO ₄ | 15m | 33 |
| GaPO ₄ ·2H ₂ O | 8m | 34 | Iron phosphate hydrate (vivianite), | | |
| Gallium samarium oxide, Ga ₅ Sm ₃ O ₁₂ | 1m | 42 | Fe ₃ (PO ₄) ₂ ·8H ₂ O | 16m | 38 |
| Gallium ytterbium oxide, Ga ₅ Yb ₃ O ₁₂ | 1m | 49 | Iron sulfate, Fe ₂ (SO ₄) ₃ | 16m | 39 |
| Gallium yttrium oxide, Ga ₅ Y ₃ O ₁₂ ... | 1m | 50 | Iron sulfate hydrate (melanterite), | | |
| Germanium, Ge | 1 | 18 | FeSO ₄ ·7H ₂ O | 8m | 38 |
| Germanium iodide, GeI ₂ | 4m | 58 | Iron sulfide (pyrite), FeS ₂ | 5 | 29 |
| Germanium(IV) iodide, GeI ₄ | 5 | 25 | Iron thorium, Fe ₁₇ Th ₂ | 12m | 67 |
| Germanium oxide, GeO ₂ (hexagonal) | | | Iron titanium oxide (ilmenite), | | |
| (low form) | 1 | 51 | FeTiO ₃ | 15m | 34 |
| | | | Lanthanum arsenate, LaAsO ₄ | 3m | 36 |

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| Lanthanum fluoride, LaF ₃ | 7 | 21 | Lithium calcium aluminum boron | | |
| Lanthanum magnesium, LaMg..... | 5m | 69 | hydroxy silicate, liddicoatite, | | |
| Lanthanum nickel platinum, | | | Ca(Li,Al) ₃ Al ₆ B ₃ Si ₆ O ₂₇ (OH) ₃ (OH,F) | 16m | 42 |
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| Lead bromide chloride, PbBrCl | 11m | 33 | Lithium niobium oxide, LiNbO ₃ | 6m | 22 |
| Lead bromide fluoride, PbBrF | 10m | 25 | Lithium nitrate, LiNO ₃ | 7 | 27 |
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| Lead carbonate (cerussite), PbCO ₃ | 2 | 56 | Li ₃ P ₃ O ₉ ·3H ₂ O | 2m | 20 |
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| Lead chromium oxide, Pb ₂ CrO ₅ | 14m | 16 | Li ₃ PO ₄ | 3m | 39 |
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| Lead fluoride, β-PbF ₂ (cubic) | 5 | 33 | Lithium selenide, Li ₂ Se | 10m | 100 |
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| tetragonal)..... | 2 | 30 | Lithium sulfate, Li ₂ SO ₄ | 6m | 26 |
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| orthorhombic)..... | 2 | 32 | Li ₂ SO ₄ ·H ₂ O | 4m | 22 |
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| Lead strontium nitrate, | | | (trigonal) | 1m | 25 |
| Pb _{.67} Sr _{.33} (NO ₃) ₂ | 12m | 53 | Lithium tungsten oxide hydrate, | | |
| Lead sulfate (anglesite), PbSO ₄ ... | 3 | 67 | Li ₂ WO ₄ ·0.5H ₂ O | 2m | 20 |
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| Lead titanium oxide (macedonite), | | | Lutetium manganese oxide, LuMnO ₃ .. | 2m | 23 |
| PbTiO ₃ | 5 | 39 | Lutetium nitride, LuN | 4m | 62 |
| Lead tungsten oxide (stolzite), | | | Lutetium oxide, Lu ₂ O ₃ | 1m | 27 |
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| Lithium aluminum fluoride, | | | Magnesium aluminum oxide (spinel), | | |
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| Lithium arsenate, Li ₃ AsO ₄ | 2m | 19 | Magnesium aluminum silicate (low | | |
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| Magnesium fluoride (sellaite), MgF_2 | 4 | 33 | Manganese chloride hydrate, $\text{MnCl}_2 \cdot 2\text{H}_2\text{O}$ | 11m | 38 |
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| Silicon oxide (α or low cristobalite), SiO_2 (tetragonal) (calculated pattern) | 15m | 180 | Sodium calcium aluminum fluoride hydrate, thomsenolite, $\text{NaCaAlF}_6 \cdot \text{H}_2\text{O}$ | 8m | 132 |
| Silicon oxide (α or low quartz), SiO_2 (hexagonal) | 3 | 24 | Sodium calcium carbonate hydrate, pirssonite, $\text{Na}_2\text{Ca}(\text{CO}_3)_2 \cdot 2\text{H}_2\text{O}$ | 9m | 106 |
| Silicon oxide (β or high cristobalite), SiO_2 (cubic) | 1 | 42 | Sodium calcium phosphate, $\beta\text{-NaCaPO}_4$ | 15m | 69 |
| Silver, Ag | 1 | 23 | Sodium calcium silicate, $\text{Na}_2\text{CaSiO}_4$ | 10m | 48 |
| Silver, Ag (reference standard) ... | 8m | 2 | Sodium calcium sulfate (glauberite), $\text{Na}_2\text{Ca}(\text{SO}_4)_2$ | 6m | 59 |
| Silver arsenate, Ag_3AsO_4 | 5 | 56 | Sodium carbonate hydrate (thermo- natrite), $\text{Na}_2\text{CO}_3 \cdot \text{H}_2\text{O}$ | 8 | 54 |
| Silver arsenic sulfide, xanthoconite, Ag_3AsS_3 | 8m | 126 | Sodium carbonate sulfate, $\text{Na}_4\text{CO}_3\text{SO}_4$ | 11m | 51 |
| Silver bromate, AgBrO_3 | 5 | 57 | Sodium carbonate sulfate (burkeite), $\text{Na}_6\text{CO}_3(\text{SO}_4)_2$ | 11m | 52 |
| Silver bromide (bromargyrite), AgBr | 4 | 46 | Sodium carbonate sulfate, $\text{Na}_6\text{CO}_3(\text{SO}_4)_2$ | 11m | 53 |
| Silver carbonate, Ag_2CO_3 | 13m | 36 | Sodium carbonate sulfate, $\text{Na}_6(\text{CO}_3)_2\text{SO}_4$ | 11m | 54 |
| Silver chlorate, AgClO_3 | 7 | 44 | Sodium chlorate, NaClO_3 | 3 | 51 |
| Silver chloride (chlorargyrite), AgCl | 4 | 44 | Sodium chlorate, NaClO_4 (orthorhombic) | 7 | 49 |
| Silver chromium oxide, Ag_2CrO_4 | 12m | 30 | Sodium chlorate hydrate, $\text{NaClO}_4 \cdot \text{H}_2\text{O}$ | 17m | 68 |
| Silver cyanide, AgCN | 9m | 48 | Sodium chloride (halite), NaCl | 2 | 41 |
| Silver fluoride, Ag_2F | 5m | 53 | Sodium chromium oxide, Na_2CrO_4 | 9m | 48 |
| Silver iodate, AgIO_4 | 9 | 49 | Sodium chromium oxide hydrate, $\text{Na}_2\text{CrO}_4 \cdot 4\text{H}_2\text{O}$ | 9m | 50 |
| Silver iodide (iodargyrite), AgI (hexagonal) | 8 | 51 | Sodium chromium oxide hydrate, $\text{Na}_2\text{Cr}_2\text{O}_7 \cdot 2\text{H}_2\text{O}$ | 7m | 62 |
| Silver iodide, $\gamma\text{-AgI}$ (cubic) | 9 | 48 | Sodium chromium oxide sulfate, $\text{Na}_4(\text{CrO}_4)(\text{SO}_4)$ | 11m | 55 |
| Silver manganese oxide, AgMnO_4 | 7m | 155 | Sodium cobalt nitrite, $\text{Na}_3\text{Co}(\text{NO}_2)_6$ | 15m | 70 |
| Silver mercury iodide, $\beta\text{-Ag}_2\text{HgI}_4$.. | 17m | 67 | Sodium cobalt(II) sulfate hydrate, $\text{Na}_2\text{Co}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ | 6m | 61 |
| Silver molybdenum oxide, Ag_2MoO_4 .. | 7 | 45 | Sodium cyanate, NaCN | 2m | 33 |
| Silver nitrate, AgNO_3 | 5 | 59 | Sodium cyanide, NaCN (cubic) | 1 | 78 |
| Silver nitrite, AgNO_2 | 5 | 60 | Sodium cyanide, NaCN (orthorhombic) at 6 °C | 1 | 79 |
| Silver oxide, Ag_2O | 1m | 45 | Sodium fluoride (villiaumite), NaF | 1 | 63 |
| Silver(II) oxide nitrate, $\text{Ag}_7\text{O}_8\text{NO}_3$ | 4 | 61 | Sodium hydrogen carbonate hydrate, trona, $\text{Na}_3\text{H}(\text{CO}_3)_2 \cdot 2\text{H}_2\text{O}$ | 15m | 71 |
| Silver phosphate, Ag_3PO_4 | 5 | 62 | Sodium hydrogen fluoride, NaHF_2 ... | 5 | 63 |
| Silver rhenium oxide, AgReO_4 | 8 | 53 | Sodium hydrogen phosphate, $\text{Na}_3\text{H}(\text{PO}_3)_4$ | 10m | 130 |
| Silver selenate, Ag_2SeO_4 | 2m | 32 | Sodium hydrogen silicate hydrate, $\text{Na}_2\text{H}_2\text{SiO}_4 \cdot 4\text{H}_2\text{O}$ | 7m | 163 |
| Silver sodium chloride, $\text{Ag}_{0.5}\text{Na}_{0.5}\text{Cl}$ | 8m | 79 | Sodium hydrogen sulfate hydrate, $\text{NaHSO}_4 \cdot \text{H}_2\text{O}$ | 9m | 52 |
| Silver sulfate, Ag_2SO_4 | 13m | 37 | Sodium hydroxide, NaOH at 300 °C .. | 4m | 69 |
| Silver sulfide (acanthite), Ag_2S .. | 10 | 51 | Sodium iodate, NaIO_3 | 7 | 47 |
| Silver terbium, AgTb | 5m | 74 | Sodium iodate, NaIO_4 | 7 | 48 |
| Silver thiocyanate, AgCNS | 16m | 62 | Sodium iodate hydrate, $\text{NaIO}_3 \cdot \text{H}_2\text{O}$.. | 17m | 73 |
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| Sodium aluminum chloride silicate, sodalite, $\text{Na}_8\text{Al}_6\text{Cl}_2(\text{SiO}_4)_6$ | 7m | 158 | | | |
| Sodium aluminum fluoride (chiolite), $\text{Na}_5\text{Al}_3\text{F}_{14}$ | 16m | 63 | | | |
| Sodium aluminum sulfate hydrate (soda alum), $\text{NaAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 15m | 68 | | | |
| Sodium azide, $\alpha\text{-NaN}_3$, at -90 to -100 °C | 8m | 129 | | | |
| Sodium azide, $\beta\text{-NaN}_3$ | 8m | 130 | | | |
| Sodium beryllium calcium aluminum fluoride oxide silicate, meliphanite, ($\text{Na}_{0.63}\text{Ca}_{1.37}\text{Be}(\text{Al}_{0.13}\text{Si}_{1.87})$ ($\text{F}_{0.75}\text{O}_{6.25}$)) | 8m | 135 | | | |

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| Sodium iron fluoride, Na_3FeF_6 | 9m | 54 | Strontium aluminum oxide, $\text{Sr}_3\text{Al}_2\text{O}_6$ | 10m | 52 |
| Sodium lanthanum fluoride silicate, $(\text{Na}_2\text{La}_8)\text{F}_2(\text{SiO}_4)_6$ | 7m | 64 | Strontium arsenate, $\text{Sr}_3(\text{AsO}_4)_2$ | 2m | 36 |
| Sodium lanthanum molybdenum oxide, $\text{NaLa}(\text{MoO}_4)_2$ | 10m | 49 | Strontium azide, $\text{Sr}(\text{N}_3)_2$ | 8m | 146 |
| Sodium magnesium aluminum boron hydroxide silicate, dravite, $\text{NaMg}_3\text{Al}_6\text{B}_3(\text{OH})_4\text{Si}_6\text{O}_{27}$ | 3m | 47 | Strontium borate, SrB_2O_4 | 3m | 53 |
| Sodium magnesium carbonate (eitelite), $\text{Na}_2\text{Mg}(\text{CO}_3)_2$ | 11m | 56 | Strontium borate, SrB_4O_7 | 4m | 36 |
| Sodium magnesium sulfate (vanthenhoffite), $\text{Na}_6\text{Mg}(\text{SO}_4)_4$ | 15m | 72 | Strontium bromate hydrate, $\text{Sr}(\text{BrO}_3)_2 \cdot \text{H}_2\text{O}$ | 17m | 76 |
| Sodium magnesium sulfate hydrate, bloodite, $\text{Na}_2\text{Mg}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ | 6m | 63 | Strontium bromide fluoride, SrBrF | 10m | 54 |
| Sodium magnesium sulfate hydrate (loewite), $\text{Na}_{12}\text{Mg}_7(\text{SO}_4)_{13} \cdot 15\text{H}_2\text{O}$ | 14m | 35 | Strontium bromide hydrate, $\text{SrBr}_2 \cdot 6\text{H}_2\text{O}$ | 4 | 60 |
| Sodium manganese(II) fluoride, NaMnF_3 | 6m | 65 | Strontium carbonate (strontianite), SrCO_3 | 3 | 56 |
| Sodium manganese sulfate hydrate, $\text{Na}_{12}\text{Mn}_7(\text{SO}_4)_{13} \cdot 15\text{H}_2\text{O}$ | 14m | 37 | Strontium chloride, SrCl_2 | 4 | 40 |
| Sodium mercury(II) chloride hydrate, $\text{NaHgCl}_3 \cdot 2\text{H}_2\text{O}$ | 6m | 66 | Strontium chloride fluoride, SrClF | 10m | 55 |
| Sodium molybdenum oxide, Na_2MoO_4 .. | 1m | 46 | Strontium chloride hydrate, $\text{SrCl}_2 \cdot 2\text{H}_2\text{O}$ | 11m | 58 |
| Sodium molybdenum oxide, $\text{Na}_2\text{Mo}_2\text{O}_7$ | 9m | 110 | Strontium chloride hydrate, $\text{SrCl}_2 \cdot 6\text{H}_2\text{O}$ | 4 | 58 |
| Sodium neodymium fluoride silicate, $(\text{Na}_2\text{Nd}_8)\text{F}_2(\text{SiO}_4)_6$ | 7m | 66 | Strontium chloride hydroxide phosphate, $\text{Sr}_5\text{Cl}_{65}(\text{OH})_{35}(\text{PO}_4)_3$ | 11m | 60 |
| Sodium nickel(II) sulfate hydrate, $\text{Na}_2\text{Ni}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ | 6m | 68 | Strontium chromium oxide, SrCr_2O_7 | 17m | 77 |
| Sodium nitrate (soda niter), NaNO_3 | 6 | 50 | Strontium chromium oxide, Sr_2CrO_4 | 16m | 71 |
| Sodium nitrite, NaNO_2 | 4 | 62 | Strontium chromium oxide hydrate, $\text{SrCr}_2\text{O}_7 \cdot 3\text{H}_2\text{O}$ | 17m | 79 |
| Sodium oxide, Na_2O | 10m | 134 | Strontium fluoride, SrF_2 | 5 | 67 |
| Sodium phosphate, $\text{Na}_3\text{P}_3\text{O}_9$ | 3m | 49 | Strontium hydroxide, $\text{Sr}(\text{OH})_2$ | 13m | 41 |
| Sodium phosphate hydrate, $\text{Na}_3\text{P}_3\text{O}_9 \cdot \text{H}_2\text{O}$ | 3m | 50 | Strontium hydroxide hydrate, $\text{Sr}(\text{OH})_2 \cdot \text{H}_2\text{O}$ | 13m | 42 |
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| Sodium phosphate hydrate, $\text{Na}_6\text{P}_6\text{O}_{18} \cdot 6\text{H}_2\text{O}$ | 5m | 54 | Strontium iodide hydrate, $\text{SrI}_2 \cdot 6\text{H}_2\text{O}$ | 8 | 58 |
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| Sodium sulfate (thenardite), Na_2SO_4 | 2 | 59 | Strontium phosphate, $\alpha\text{-Sr}_2\text{P}_2\text{O}_7$ | 11m | 62 |
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| Sodium sulfide, Na_2S | 10m | 140 | Strontium scandium oxide hydrate, $\text{Sr}_3\text{Sc}_2\text{O}_6 \cdot 6\text{H}_2\text{O}$ | 6m | 78 |
| Sodium sulfite, Na_2SO_3 | 3 | 60 | Strontium silicate, Sr_3SiO_5 | 13m | 44 |
| Sodium telluride, Na_2Te | 10m | 141 | Strontium sulfate (celestite), SrSO_4 | 2 | 61 |
| Sodium tin fluoride, NaSn_2F_5 | 7m | 166 | Strontium sulfide, SrS | 7 | 52 |
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| Sodium zinc sulfate hydrate, $\text{Na}_2\text{Zn}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ | 6m | 72 | Strontium tungsten oxide, Sr_2WO_5 .. | 12m | 32 |
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| | | | Sulfamic acid, $\text{H}_2\text{NSO}_3\text{H}$ | 7 | 54 |
| | | | Sulfur, S (orthorhombic) | 9 | 54 |
| | | | Tantalum, Ta | 1 | 29 |
| | | | Tantalum silicide, TaSi_2 | 8 | 59 |
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| | | | Yttrium telluride, YTe | 4m | 75 |
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| | | | Zinc ammine chloride, Zn(NH ₃) ₂ Cl ₂ | 10m | 59 |
| | | | Zinc antimony oxide, ZnSb ₂ O ₄ | 4m | 39 |
| | | | Zinc borate, Zn ₄ B ₆ O ₁₃ | 13m | 48 |
| | | | Zinc carbonate, smithsonite, ZnCO ₃ | 8 | 69 |
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| Zinc tin oxide, Zn_2SnO_4 | 10m | 62 |
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| C ₅ H ₇ NO ₄ Zn·2H ₂ O | Zinc glutamate hydrate | 7m | 170 |
| C ₅ H ₈ NNaO ₄ ·H ₂ O | Sodium glutamate hydrate | 17m | 70 |
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| C ₆ H ₁₂ O ₆ | α-D-Glucose | 11m | 28 |
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| 4-Acetyl-2'-fluorodiphenyl | $C_{14}H_{11}FO$ | 8m | 91 |
| Alanine, L- | $CH_3CHNH_2CO_2H$ | 8m | 93 |
| Allobarbitol | $C_{10}H_{12}N_2O_3$ | 14m | 41 |
| Amobarbital, form I, | $C_{11}H_{18}N_2O_3$ | 15m | 114 |
| Amobarbital, form II | $C_{11}H_{18}N_2O_3$ | 15m | 117 |
| Ammonium acetate | $NH_4 \cdot CH_3CO_2$ | 8m | 95 |
| Ammonium formate | NH_4HCO_2 | 11m | 9 |
| Ammonium oxalate hydrate (oxammite) | $(NH_4)_2C_2O_4 \cdot H_2O$ | 7 | 5 |
| Ammonium yttrium oxalate hydrate | $NH_4Y(C_2O_4)_2 \cdot H_2O$ | 8m | 97 |
| Amphetamine sulfate, (+)- | $C_{18}H_{28}N_2O_4S$ | 15m | 119 |
| p-Anisic acid | $C_8H_8O_3$ | 16m | 11 |
| Ascorbic acid, L- | $C_6H_8O_6$ | 8m | 99 |
| Azobenzene | $C_6H_5NNC_6H_5$ | 7m | 86 |
| Barbital, form I, | $C_8H_{12}N_2O_3$ | 15m | 126 |
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| Barbital, form IV, | $C_8H_{12}N_2O_3$ | 15m | 130 |
| Benactyzine hydrochloride | $C_{20}H_{26}ClNO_3$ | 16m | 92 |
| o-Bromobenzoic acid | $C_7H_5BrO_2$ | 16m | 22 |
| Bufotenine | $C_{12}H_{16}N_2O$ | 15m | 133 |
| Cadmium hexamidazole nitrate | $Cd(C_3H_4N_2)_6(NO_3)_2$ | 8m | 23 |
| Calcium formate | $Ca(HCO_2)_2$ | 8 | 16 |
| Calcium malate hydrate, | $Ca(O_2C)_2(CH_2CHOH) \cdot 2H_2O$ | 10m | 76 |
| Cannabidiol | $C_{21}H_{30}O_2$ | 16m | 111 |
| m-Chlorobenzoic acid | $C_7H_5ClO_2$ | 16m | 30 |
| Chlorpromazine | $C_{17}H_{19}ClN_2S$ | 14m | 60 |
| Cinchonine | $C_{19}H_{22}N_2O$ | 17m | 26 |
| Clophenixol hydrate | $C_{22}H_{25}ClN_2OS \cdot 2H_2O$ | 17m | 28 |
| Cobalt acetate hydrate | $Co(C_2H_3O_2)_2 \cdot 4H_2O$ | 12m | 19 |
| Cocaine hydrochloride, L- | $C_{17}H_{22}ClNO_4$ | 16m | 114 |
| Codeine hydrobromide hydrate | $C_{18}H_{22}BrNO_3 \cdot 2H_2O$ | 16m | 117 |
| Copper glutamate hydrate | $Cu(O_2C)_2(H_2NCHCH_2CH_2) \cdot 2H_2O$ | 7m | 110 |
| Copper tetraimidazole nitrate | $Cu(C_3H_4N_2)_4(NO_3)_2$ | 13m | 24 |
| Copper tetrapyrazole chloride | $Cu(C_3H_4N_2)_4Cl_2$ | 8m | 31 |
| Creatinine | $C_4H_7N_3O$ | 15m | 31 |
| Cysteine, L- | $HSCH_2 \cdot CH(NH_2) \cdot COOH$ | 11m | 86 |
| Dextrose | $C_6H_{12}O_6$ | 11m | 28 |
| Diazepam | $C_{16}H_{13}ClN_2O$ | 14m | 106 |
| Dibenzoylmethane | $(C_6H_5CO)_2CH_2$ | 7m | 115 |
| α -Dihydrophyllocladene, hartite (or bombiccite) | $C_{20}H_{34}$ | 16m | 122 |
| (N,N)-Dimethyltryptamine | $C_{12}H_{16}N_2$ | 14m | 109 |
| bis-(o-Dodecacarborane) | $C_{4}B_{26}H_{22}$ | 6m | 7 |
| Ephedrine hydrochloride, (-)- | $C_{10}H_{16}ClNO$ | 16m | 124 |
| p-Fluorobenzoic acid | $C_7H_5FO_2$ | 16m | 36 |
| Glucose, α -D- | $C_6H_{12}O_6$ | 11m | 28 |
| Glutamic acid, β -L- | $C_5H_9NO_4$ | 17m | 32 |
| α -Glycine | $C_2H_5NO_2$ | 17m | 34 |
| Glyoxime | $H_2C_2(NO_2)_2$ | 8m | 102 |
| Guanidinium chloride | $CH_5N_3 \cdot HCl$ | 17m | 35 |
| Haloperidol | $C_{21}H_{23}ClFNO_2$ | 16m | 127 |
| Hexamethylenediammonium adipate, | $(CH_2)_4(CO_2H_3N)_2(CH_2)_6$ | 7m | 121 |
| Hexamethylenetetramine | $C_6H_{12}N_4$ | 17m | 37 |
| α -HMX | $C_4H_8N_8O_8$ | 11m | 100 |
| β -HMX | $C_4H_8N_8O_8$ | 11m | 102 |
| Holmium ethylsulfate hydrate | $Ho[(C_2H_5)SO_4]_3 \cdot 9H_2O$ | 1m | 18 |
| γ -Hydroquinone | HOC_6H_4OH | 8m | 107 |
| Imipramine hydrochloride | $C_{19}H_{25}ClN_2$ | 16m | 129 |
| Iron oxalate hydrate (humboldtine) | $FeC_2O_4 \cdot 2H_2O$ | 10m | 24 |
| Lead formate | $Pb(HCO_2)_2$ | 8 | 30 |
| Lithium oxalate | $Li_2C_2O_4$ | 10m | 34 |

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| Mercury acetate | $C_4H_6Hg_2O_4$ | 17m | 51 |
| Mercury o-phthalate | $C_6H_4(CO_2Hg)_2$ | 10m | 113 |
| Methapyrilene hydrochloride, | $C_{14}H_{20}ClN_3S$ | 14m | 112 |
| Metharbital | $C_9H_{14}N_2O_3$ | 15m | 177 |
| Methyl sulfonanilide | $C_6H_5NHSO_2CH_3$ | 9m | 78 |
| N-Methylphenazinium-7,7,8,8-tetra- cyanoquinodimethanide | $C_{25}H_{15}N_6$ | 7m | 146 |
| Morphine hydrochloride hydrate | $C_{17}H_{20}ClNO_3 \cdot 3H_2O$ | 16m | 133 |
| Naloxone hydrochloride hydrate | $C_{19}H_{22}ClNO_4 \cdot 2H_2O$ | 16m | 136 |
| 2-Naphthylamine, N-phenyl- | $C_{10}H_7NHC_6H_5$ | 6m | 29 |
| Neodymium ethylsulfate hydrate | $Nd[(C_2H_5)SO_4]_3 \cdot 9H_2O$ | 9 | 41 |
| Nickel acetate hydrate | $Ni(C_2H_3O_2)_2 \cdot 4H_2O$ | 13m | 31 |
| Nickel hexaimidazole nitrate | $Ni(C_3H_4N_2)_6(NO_3)_2$ | 7m | 27 |
| Nickel tetrapyrazole chloride | $Ni(C_3H_4N_2)_4Cl_2$ | 8m | 44 |
| Nicotinic acid | $C_6H_5NO_2$ | 16m | 54 |
| Octahydro-1,3,5,7-tetranitro- 1,3,5,7-tetrazocine (α -HMX) | $C_4H_8N_8O_8$ | 11m | 100 |
| Octahydro-1,3,5,7-tetranitro- 1,3,5,7-tetrazocine (β -HMX) | $C_4H_8N_8O_8$ | 11m | 102 |
| Oxalic acid hydrate | $C_2H_2O_4 \cdot 2H_2O$ | 16m | 55 |
| Palladium bis-(N-isopropyl-3- ethylsalicylaldiminate), | $Pd(C_{12}H_{16}NO)_2$ | 7m | 144 |
| Pentaerythritol | $C_5H_{12}O_4$ | 17m | 55 |
| Phencyclidine hydrochloride | $C_{17}H_{26}ClN$ | 16m | 141 |
| Phenobarbital, form III | $C_{12}H_{12}N_2O_3$ | 16m | 144 |
| Phenylhydrazine hydrochloride | $C_6H_8N_2 \cdot HCl$ | 17m | 55 |
| Picric acid | $C_6H_3N_3O_7$ | 16m | 56 |
| Pimelic acid | $(CH_2)_5(CO_2H)_2$ | 7m | 153 |
| Potassium formate-formic acid complex | $KO_2CH \cdot HO_2CH$ | 9m | 93 |
| Potassium hydrogen o-phthalate, | $C_6H_4(COOH)(COOK)$ | 4m | 30 |
| Potassium hydrogen oxalate hydrate | $C_4H_3KO_8 \cdot 2H_2O$ | 17m | 60 |
| Potassium oxalate hydrate | $K_2C_2O_4 \cdot H_2O$ | 9m | 39 |
| Potassium oxalate perhydrate | $K_2C_2O_4 \cdot H_2O_2$ | 9m | 96 |
| Potassium sodium tartrate hydrate | $C_4H_4KNaO_6 \cdot 4H_2O$ | 15m | 55 |
| Procaine hydrochloride | $C_{13}H_{21}ClN_2O_2$ | 16m | 149 |
| Psilocin | $C_{12}H_{16}N_2O$ | 16m | 152 |
| Psilocybin methanolate | $C_{13}H_{21}N_2O_4P$ | 16m | 154 |
| Reserpine | $C_{33}H_{40}N_2O_9$ | 8m | 123 |
| Rubidium oxalate perhydrate | $Rb_2C_2O_4 \cdot H_2O_2$ | 9m | 102 |
| Silver oxalate | $Ag_2C_2O_4$ | 9m | 47 |
| Sodium acetate hydrate | $C_2H_3NaO_2 \cdot 3H_2O$ | 15m | 66 |
| Sodium barbital | $C_8H_{11}N_2NaO_3$ | 16m | 157 |
| Sodium glutamate hydrate | $C_5H_8NNaO_4 \cdot H_2O$ | 17m | 70 |
| Sodium hydrogen oxalate hydrate | $C_2HNaO_4 \cdot H_2O$ | 17m | 72 |
| Sodium oxalate | $Na_2C_2O_4$ | 6m | 70 |
| Sodium D-tartrate hydrate | $(CHOH-CO_2Na)_2 \cdot 2H_2O$ | 11m | 110 |
| Strontium formate | $Sr(CHO_2)_2$ | 8 | 55 |
| Strontium formate hydrate | $Sr(CHO_2)_2 \cdot 2H_2O$ (orthorhombic) | 8 | 56 |
| Sucrose | $C_{12}H_{22}O_{11}$ | 11m | 66 |
| Tartaric acid, D- | $(CHOHCO_2H)_2$ | 7m | 168 |
| Δ^9 -Tetrahydrocannabinolic acid B | $C_{22}H_{30}O_4$ | 16m | 160 |
| Thallium hydrogen phthalate | $C_8H_5O_4Tl$ | 16m | 75 |
| Thiosemicarbazide | CH_5N_3S | 17m | 81 |
| Thiourea | CH_4N_2S | 17m | 83 |
| Trimethylammonium chloride | $(CH_3)_3NHCl$ | 9m | 113 |
| 2,4,6-Trinitrophenetole | $C_2H_5OC_6H_2(NO_2)_3$ | 8m | 152 |
| Urea | $CO(NH_2)_2$ | 7 | 61 |
| Uric acid, phase I, (calc. pattern) | $C_5H_4N_4O_3$ | 8m | 154 |
| Uric acid (phase I) | $C_5H_4N_4O_3$ | 16m | 78 |
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Handbooks—Recommended codes of engineering and industrial practice (including safety codes) developed in cooperation with interested industries, professional organizations, and regulatory bodies.

Special Publications—Include proceedings of conferences sponsored by NBS, NBS annual reports, and other special publications appropriate to this grouping such as wall charts, pocket cards, and bibliographies.

Applied Mathematics Series—Mathematical tables, manuals, and studies of special interest to physicists, engineers, chemists, biologists, mathematicians, computer programmers, and others engaged in scientific and technical work.

National Standard Reference Data Series—Provides quantitative data on the physical and chemical properties of materials, compiled from the world's literature and critically evaluated. Developed under a worldwide program coordinated by NBS under the authority of the National Standard Data Act (Public Law 90-396).

NOTE: The principal publication outlet for the foregoing data is the Journal of Physical and Chemical Reference Data (JPCRD) published quarterly for NBS by the American Chemical Society (ACS) and the American Institute of Physics (AIP). Subscriptions, reprints, and supplements available from ACS, 1155 Sixteenth St., NW, Washington, DC 20056.

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NBS Interagency Reports (NBSIR)—A special series of interim or final reports on work performed by NBS for outside sponsors (both government and non-government). In general, initial distribution is handled by the sponsor; public distribution is by the National Technical Information Services, Springfield, VA 22161, in paper copy or microfiche form.

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